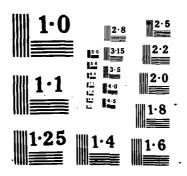
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update of an Efficient Computer Code (NLTE) to Calculate Emission and Transmission of Radiation Through Non-Equilibrium Atmospheres

P. P. WINTERSTEINER

R. D. SHARMA



20 September 1985







INFRARED TECHNOLOGY DIVISION

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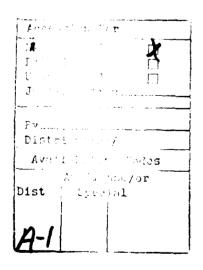
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Update of an Efficient Computer Code (NLTE) to Calculate Emission and Transmission of Radiation Through Non-Equilibrium Atmospheres

1. INTRODUCTION

The Air Force Geophysics Laboratory (AFGL) is in the process of developing comprehensive FORTRAN codes for calculating the radiance due to infrared-active species in the upper atmosphere. The objective of this work is to improve the understanding of the physics and chemistry of the upper atmosphere. In particular, the codes deal with atmospheric conditions in which local thermodynamic equilibrium (I.TE) cannot be assumed; that is, conditions under which the populations of ro-vibrational states cannot (necessarily) be given by a Beltzmann distribution with the kinetic temperature.

This report describes program NLTE, which is a general line-by-line code predicting the infrared radiance from individual molecular species at an observing site located within the upper atmosphere or in limb geometry viewing from outside the atmosphere. The present version of the program assumes that lines do not overlap to an appreciable extent and that there are no lateral variations in the atmosphere. It operates in a stand-alone mode and also is being incorporated into a larger package for use in iterative or repetitive applications. Emphasis has been placed upon (1) achieving accurate results at all steps of this detailed calcu-

⁽Received for publication 16 September 1985)

lation, and (2) making the program easy to use and transportable. Since its first release, ¹ NLTE has undergone substantial revisions which make it much faster and give it more capabilities, and which, therefore, necessitate a new release and this accompanying report.

The program output consists of the total radiance (watt/cm 2 -ster) for a specified vibrational band for a set of viewing paths, and also the spectral radiance (watt/cm 2 -ster- μ m or watt/cm 2 -ster-cm $^{-1}$) if an instrumental resolution parameter is provided. The band radiance is just the sum of the integrated radiance for all the individual lines. If a single ro-vibrational transition, rather than an entire band, is requested, the program gives the integrated line radiance and also many intermediate results, including the detailed spectral radiance profile for the line.

NLTE requires the user to prepare three input files. They specify (1) the molecule, isotope, and band under consideration, and the viewing geometry; (2) the atmospheric profile; and (3) an appropriate subset of the AFGL Atmospheric Absorption Line Parameters Compilation. ^{2,3,4} In the case of the second file, the quantities required for an altitude range sufficient to complete the calculation are

- (a) the kinetic temperature, T,
- (b) the total number density and a vibrational temperature characterizing the the upper level of the band under consideration (and, for hot bands, the lower level as well) or equivalent information, and
- (c) a vibrational temperature for the lowest-lying excited state for use a calculating the vibrational partition function, or equivalent information. "Equivalent information" for both (b) and (c) consists of number densities of lower and upper vibrational levels. The third file is necessary because it provides the properties of the individual ro-vibrational transitions, which are needed to determine the absorption and reradiation of energy by each line in the wavelength region under consideration.

Sharma, R.D., Siani, R., Bullitt, M., and Wintersteiner, P.P. (1983) A
 <u>Computer Code to Calculate Emission and Transmission of Infrared Radiation Through a Non-Equilibrium Atmosphere</u>, AFGL-TR-83-0168, ADA 137162.

McClatchey, R.A., Benedict, W.S., Clough, S.A., Burch, D.E., Calfee, R.F., Fox, K., Rothman, L.S., and Garing, J.S. (1973) <u>AFCRL Atmospheric Absorption Line Parameters Compilation</u>, AFCRL-TR-73-0096, AD 762904.

Rothman, L.S., Gamache, R.R., Barbe, A., Goldman, A., Gillis, J.R., Brown, L.R., Toth, R.A., Flaud, J.M., and Camy-Payret, C. (1983) AFGL atmospheric absorption line parameters compilation: 1982 edition, Appl. Opt. 22:2247.

Rothman, L.S., Goldman, A., Gillis, J.R., Gamache, R.R., Pickett, H.M., Poynter, R.L., Husson, N., and Chedin, A. (1983) AFGL trace gas compilation: 1982 edition, <u>Appl. Opt.</u> 22:261

Section 2 of this report gives the formulation of the problem and the algorithms employed in its solution. Section 3 describes how to use the code, and Section 4 gives examples of some of the results obtained to date. The appendixes contain the source code and sample program output.

2. FORMULATION

2.1 Radiative Transfer Problem

The problem of radiative transport along a viewing path within an absorbing and emitting medium is formulated most generally 5 in terms of the equation of transfer.

$$\frac{1}{k_{\mathcal{V}}(s)\rho(s)} \frac{dI_{\mathcal{V}}(s)}{ds} = J_{\mathcal{V}}(s) - I_{\mathcal{V}}(s)$$
 (1)

and whatever boundary conditions are appropriate. In this equation, both I_{ν} , which is the specific intensity of radiation at wavenumber ν , and J_{ν} , the source function, have units of watts/(cm²-ster-cm⁻¹) or equivalent units (for example, photons/sec instead of watts, micrometers instead of cm⁻¹). The viewing path is parameterized by the position variable, s. The absorption coefficient (cm²/molecule) and the total number density (molecules/cm³) of the molecular specie in question are, respectively, k_{ν} and ρ . Furthermore, the optical depth between an observation point s and a reference point s' is defined by a line integral over the viewing path:

$$\tau_{\boldsymbol{v}}(\mathbf{s},\mathbf{s}') = \int_{\mathbf{s}'}^{\mathbf{s}} \mathbf{k}_{\boldsymbol{v}}(\mathbf{s}'') \rho(\mathbf{s}'') d\mathbf{s}''$$
 (2)

In the problem we are presently considering, the only processes of interest within the atmosphere are stimulated and spontaneous emission from molecules in the excited state of the transition in question, and absorption by molecules in the corresponding lower state. That is, scattering into and out of the beam is neglected. The equation of transfer for this case can thus be derived directly from the three Einstein coefficients and the populations of the upper and lower

^{5.} Chandrasekhar, S. (1960) Radiative Transfer, Dover, New York.

radiating states. Using the relations between these coefficients, 6 we arrived at 1

$$\frac{\mathrm{d}I_{\nu}(s)}{\mathrm{d}s} = \frac{\mathrm{h}\nu_{o}}{\mathrm{c}} B_{\ell u} f_{\nu}(s) n_{\ell}(s) \left[2\mathrm{c}\nu_{o}^{2} \gamma(s) - I_{\nu}(s) (1 - \gamma(s)) \right]$$
(3)

where the position-dependence is written explicitly and the frequency-dependence is indicated by the subscript ν . In this equation, n_{ℓ} is the lower-state number density, f_{ν} is the normalized lineshape of the absorption coefficient, $B_{\ell u}$ is the Einstein coefficient for absorption, ν_0 is the resonant frequency in wave-numbers, h is Planck's constant, c is the speed of light, and γ is given by

$$\gamma(s) = \frac{g_{\ell} n_{\mathbf{u}}(s)}{g_{\mathbf{u}} n_{\ell}(s)}$$
 (4)

where the g's are statistical weights of the upper (u) and lower (ℓ) radiating states and the n's are the number densities. The (1- γ) factor in Eq. (3) accounts for stimulated emission.

By "normalized lineshape," we mean that f_{ν} satisfies

$$\int_{-\infty}^{\infty} f_{\nu} \, \mathrm{d}\nu \quad \approx \quad 1 \tag{5}$$

In NLTE, the Voigt profile is used for f_{ν} , although the user can specify a Doppler lineshape if necessary.

The correspondence between Eqs. (1) and (3) reveals that the absorption coefficient is given by

$$k_{\nu}(s) = \frac{h\nu_{0}}{c} B_{\ell u} f_{\nu}(s) \frac{n_{\ell}(s)}{\rho(s)} (1 - \gamma(s))$$
(6)

and the source function by

$$J_{\nu}(s) = 2c\nu_{o}^{2} \frac{\gamma(s)}{1 - \gamma(s)}$$
 (7)

Penner, S.S. (1959) Quantitative Molecular Spectroscopy and Gas Emissivities, Addison-Wesley, London.

The absence of an explicit frequency-dependence is proper for this particular source function. The emission coefficient, $j\nu$, which has the same units as the absorption coefficient and plays an analogous role, contains the frequency-dependence and is given by

$$j_{\nu} = k_{\nu} J_{\nu} \tag{8}$$

The boundary conditions for the problem can be determined from the allowed viewing paths, which are shown in Figure 1. Since the paths begin above the atmosphere, the intensity $I_{\nu}(s')$ must be zero for all frequencies unless the line-of-sight intersects the sun, or else some other zodiacal contribution is not negligible. In either case, this contribution can be separated completely from the atmospheric emission and treat ' - mple attenuation problem, so we do not discuss it further in this deathers.

2.2 Formal Solution

With this particular boundary constraint, the formal solution of Eq. (1) for the line-of-sight path extending from s' to the observer at s can be written as

$$I_{\nu}(s) = \int_{s'}^{s} J_{\nu}(s'') k_{\nu}(s'') \rho(s'') e^{-\tau_{\nu}(s, s'')} ds''$$
(9)

With the help of Eqs. (4-8) and the relation between $B_{\ell\,u}$ and the Einstein A coefficient,

$$A = 8\pi h \nu_0^3 \frac{g_{\ell}}{g_{u}} B_{\ell u}$$
 (10)

it is transformed to

$$I_{\nu}(s) = \int_{s'}^{s} j_{\nu}(s'') \rho(s'') e^{-\tau} \nu^{(s, s'')} ds''$$

$$= \frac{A}{4\pi} \int_{s'}^{s} n_{u}(s'') f_{\nu}(s'') e^{-\tau} \nu^{(s, s'')} ds''$$
(11)

The first form of Eq. (11) expresses the facts that (1) an amount of radiant energy,

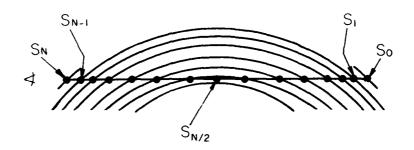


Figure 1a. Limb Viewing Path in a Layered Atmosphere. s_0 is the beginning of the path, $s_N^{\ /2}$ is the tangent point, and $s_N^{\ }$ is the location of the observer. In the text, s_0 and $s_N^{\ }$ are referred to as s' and s, respectively

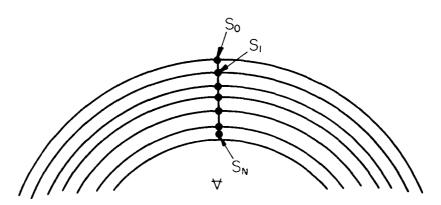


Figure 1b. Zenith Viewing Path in a Layered Atmosphere

 j_{ν} , emitted per molecule at frequency ν at the point s' along the path (per cm per ster) is reduced by an amount (the exponential) determined by the optical depth between that point and the observer at s; and (2) that the total radiance due to all points s' between s' and s is just the total (integral) contribution from all such points weighted by the total number of emitters. The second integral expresses the same thing in slightly different terms: the volume emission rate (photons/sec - cm - ster - cm - 1) is simply $An_uf_{\nu}/4\pi$.

Bullitt et al ⁷ have further transformed the formal solution into expressions that make it easy to visualize how the complicated single-line radiance profiles

Bullitt, M.K., Bakshi, P.M., Picard, R.H., and Sharma, R.D. (1985) Numerical and analytical study of high-resolution limb spectral radiance from non-equilibrium atmospheres, <u>J. Quant. Spectrosc. and Rad. Transfer</u>, 34:33.

evolve, and that also lead to some useful analytical approximations. They make the definitions

$$F_{\nu}(s, s'') = k_{\nu}(s'') \rho(s'') e^{-\tau_{\nu}(s, s'')}$$
 (12)

$$R(s) = 2c \nu_0^2 \frac{\gamma(s)}{1 - \gamma(s)}. \qquad (13)$$

R is just the source function, and F_{ν} serves as a weighting function for the path when the radiance at the observation point is written as

$$I_{\nu}(s) = \int_{s'}^{s} R(s'') F_{\nu}(s, s'') ds''$$
 (14)

This form is intrinsically no simpler than the others; we introduce it because we later make use of arguments which most easily are expressed in terms of the quantity R.

2.3 NLTE Algorithm

2.3.1 LAYERING

Our prescription for solving for the radiance relies upon the assumption that a stratified model atmosphere consisting of homogeneous concentric layers (see Figure 1) can be made into a sufficiently accurate representation of the actual atmosphere to produce correct results. In NLTE, the altitude grid is defined by whatever altitudes are read on the atmospheric profile data file. The properties of the layers are then determined from the pairs of grid points bounding each of them. In the case of temperatures, the average value is used; in the case of number densities, the mean square value is used. For example, for the ith layer

$$T_{i} = \frac{1}{2} \left[T(s_{i}) + T(s_{i+1}) \right]$$
 (15a)

$$\rho_{i} = \left[\rho(s_{i}) \rho(s_{i+1}) \right]^{1/2}$$
 (15b)

It is understood that each position s along the viewing path is associated with an altitude, h, which is really the correct parameter for the physical properties of the atmosphere.

2.3.2 OPTICAL DEPTH

The optical depth at frequency ν is obviously an important quantity for the radiance calculation. In order to calculate it numerically, we must correlate the Einstein absorption coefficient with the information contained in the AFGL database, anamely the line strength S(T_S) evaluated under conditions of LTE at the standard temperature, T_S = 296 K. For arbitrary conditions, the line strength S satisfies

$$Sf_{\nu} = k_{\nu} \tag{16}$$

and in fact is equal to the absorption coefficient integrated over ν . The connection with the Einstein absorption coefficient is made through Eq. (6), in which the ratio n $_{\ell}/\rho$ is simply the probability, P_{ℓ} , that the lower ro-vibrational state be occupied under the specified conditions. It follows that

$$\frac{h\nu_{o}}{c} B_{\ell u} = \frac{S(T_{s})}{P_{\ell}(T_{s}, T_{s})} \left(1 - e^{-c_{2}\nu_{o}/T_{s}}\right)^{-1}$$
(17)

where S, P_{ℓ} , and $(1-\gamma)$ are evaluated for conditions of LTE at the temperature T_s . c_2 is the second radiation constant. Then, for arbitrary conditions, one can plug Eq. (17) into Eq. (6) and use Eq. (16) in Eq. (2) to derive the optical depth along the path within the ith homogeneous layer as

$$\tau_{\boldsymbol{\nu}} (\mathbf{s}_{i+1}, \mathbf{s}_{i}) = \Delta \tau_{\boldsymbol{\nu} i}$$

$$= S(\mathbf{T}_{s}) \frac{P_{\ell} (\mathbf{T}_{i}, \mathbf{T}_{vi})}{P_{\ell} (\mathbf{T}_{c}, \mathbf{T}_{c})} \frac{1 - \gamma_{i}}{1 - \exp(-\mathbf{c}_{2} \boldsymbol{\nu}_{c}/\mathbf{T}_{c})} f_{\boldsymbol{\nu} i} \rho_{i} \Delta \mathbf{s}_{i}$$
(18)

The notation we have adopted here is that the subscript i on each quantity replaces the independent variable, s, and implies a constant value within the ith layer. Also, $\Delta s = s_{i+1} - s_i$. For general conditions, the probability that the lower state be occupied depends on the vibrational and rotational temperatures, T_v and T_R , for the state in question. We regard all rotational temperatures as equal to the kinetic temperature, however, so, in general

$$P_{\ell}(T, T_{v}'') = \alpha_{i} g_{\ell} \frac{\exp(-c_{2} E_{v}''/T_{v}'')}{Q_{v}(T_{v}'')} \frac{\exp(-c_{2} E_{R}''/T)}{Q_{R}(T)}$$
(19)

where E $_v$ and E $_R$ are the vibrational and rotational energies of the lower state in wavenumbers, T $_v$ and T are the vibrational and rotational temperatures describing the lower state, Q $_v$ and Q $_R$ are the vibrational and rotational partition functions, c $_2$ is the second radiation constant, and α_I is the isotopic abundance expressed as a fraction of the total, so that

$$\sum_{\mathbf{I}} \alpha_{\mathbf{I}} = 1. \tag{20}$$

The partition functions are, of course, evaluated for the conditions at hand. The particular band vibrational temperature, T_v ', may not be sufficient to determine Q_v , however. We defer a discussion of the means of approximating them until Section 2.3.7.

2.3.3 RADIANCE

Division of the viewing path into segments (s_i, s_{i+1}) as indicated in Figure 1 does not alter the exact nature of the solution in Eq. (14):

$$I_{\nu}(s) = \sum_{i=0}^{N-1} \int_{s_i}^{s_{i+1}} R(s'') F_{\nu}(s, s'') ds''$$
 (21)

The first approximation is to let $R(s^{\prime\prime})$ be a constant over each segment, in accordance with our assumption of homogeneous layers. Then

$$I_{\nu}(s) \stackrel{\sim}{=} \sum_{i=0}^{N-1} R_{i} \int_{s_{i}}^{s_{i+1}} F_{\nu}(s, s'') ds''$$
(22)

However, by the definitions made in Eq. (12) and Eq. (2), F_{ν} is a perfect differential equal to

$$F_{\nu}(s,s'') = -\frac{d\tau_{\nu}(s,s'')}{ds''}e^{-\tau_{\nu}(s,s'')} = \frac{d}{ds''}\left[e^{-\tau_{\nu}(s,s'')}\right]$$
 (23)

This leads to

$$I_{\nu}(s) \cong \sum_{i=0}^{N-1} R_{i} e^{-\tau_{\nu} (s, s_{i+1})} \left[1 - \exp(-\Delta \tau_{\nu i}) \right]$$
 (24)

with $\Delta \tau_{\nu\, i}$ given by Eq. (18). Moreover, the fact that the optical depth along the path segments is additive, so that

$$\tau_{\nu} (s, s_{i+1}) = \sum_{j=i+1}^{N-1} \Delta \tau_{\nu j},$$
 (25)

leads to the result

$$I_{\nu}(s) \simeq \sum_{i=0}^{N-1} R_{i} \left[1 - \exp\left(-\Delta \tau_{\nu i}\right) \right] \exp \left[-\sum_{j=i+1}^{N-1} \Delta \tau_{\nu j} \right]$$
 (26)

The only approximations involved here are taking R, ${\bf F}_{\nu}$, and ${\bf n}_{u}$ to be constants within each layer.

One can see that one series is embedded within the other in Eq. (26). It is not necessary, however, to separately evaluate two series for each frequency. One can obtain the desired sum starting with i = 0 (the farthest layer) with the following algorithm:

Define
$$E_{i} = \exp(-\Delta \tau_{\nu i})$$

$$X_{i} = R_{i}[1 - E_{i}]$$
Calculate
$$P_{o} = X_{o}$$

$$P_{i} = X_{i} + P_{i-1}E_{i}$$

$$i = 1, 2, \dots, N-1$$
Set
$$I_{\nu}(s) = P_{N-1}$$

 $\mathbf{E_i}$ represents the amount by which a unit of radiation is attenuated in passing completely through layer i, and $\mathbf{X_i}$ is the amount of radiation from the ith layer alone appearing on the observer's side of that layer. The P's represent the total radiation appearing at each boundary. An alternative but completely equivalent algorithm is given by

Define
$$\begin{array}{ccc} \mathbf{E_i} &=& \exp{(-\Delta \tau_{\nu\,i})} \\ \mathbf{X_i} &=& \mathbf{R_i} [1-\mathbf{E_i}] \\ \mathbf{Q_{N-1}} &=& 1 \end{array}$$
 Calculate
$$\begin{array}{cccc} \mathbf{Q_{i-1}} &=& \mathbf{Q_i} \mathbf{E_i} \\ \mathbf{P_i} &=& \mathbf{Q_i} \mathbf{X_i} \end{array}$$

Evaluate
$$I_{\nu}(s) = \sum_{i=N-1}^{o} P_{i}$$

The only difference in these two approaches is the order in which the atmospheric layers are treated. In the second algorithm, Q_i is the total transmittance from the near side of the ith layer to the observer and P_i is the contribution at the observer's location from the ith layer alone. The advantage of this approach is that one can cut off the summation whenever the attenuation becomes severe enough to negate contributions from ever more distant layers. That is, the summation need not be carried as far as i = 0. Obviously, such a truncation is not possible in the first algorithm. The second algorithm, which is especially useful when the observer is within the atmosphere (for example, zenith-look) has been incorporated into NLTE.

2.3.4 INTEGRATED RADIANCE

The quantity which is the main objective of these calculations is obtained by integrating the radiance profiles over frequency. For each line, one evaluates

$$I(s) = \int_{-\infty}^{\infty} I_{\nu}(s) d\nu$$
 (27)

For a band, NLTE sums the results over individual lines.

Figure 2 gives some typical single-line radiance profiles for limb geometry, using lines from the ν_2 fundamental of ${\rm CO}_2$ near $15\mu{\rm m}$. Several of the lines are severely self-absorbed along this path, which has a tangent height of 70 km. The weakest lines mimic Doppler lines; stronger lines decrease monotonically from the center but have much more pronounced wings; and the strongest lines have maxima and possibly minima away from the line center, as well as wings where the function decreases smoothly and monotonically, but very slowly, over a very large range of frequencies.

Figure 3 gives the vibrational and kinetic temperatures used in the calculation of these profiles.

For each line, NLTE evaluates Eq. (27) using an analytical approximation which is valid only when the path optical depth is less than unity at the line center. This approximation may be accepted as an appropriate value for I(s) if a "thin-line" criterion, described in Section 2.3.4.2, is satisfied. Otherwise, the integral is evaluated numerically using the "thick-line" procedure described in Section 2.3.4.1. Because of the heavy computational requirements of the thick-line procedures, the program bypasses it whenever the thin-line approximation is sufficiently accurate.

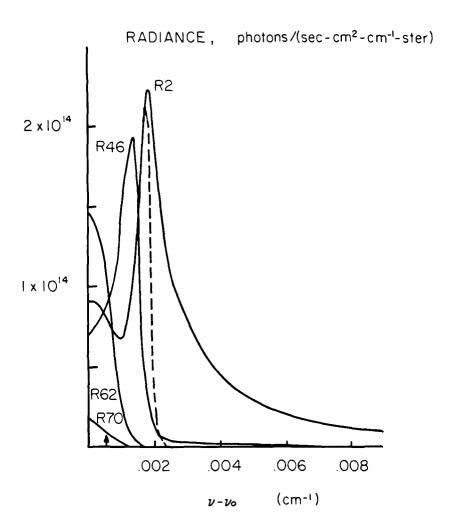


Figure 2. Radiance Profiles of Four Lines of the R Branch of the CO₂ (ν_2) Fundamental, Using Limb Geometry and a Tangent Height of 70 km. The dotted line is the R2 profile assuming a Doppler rather than Voigt lineshape. The arrow indicates the Doppler linewidth at 70 km.

2.3.4.1 Thick-Line Algorithm

When the thin-line approximation is unacceptable, Eq. (27) is evaluated numerically over a range between $\nu_{\rm O}$ and a certain cutoff frequency $\nu_{\rm C}$, and the contribution from the region between $\nu_{\rm C}$ and infinity is approximated by an analytical expression. Since I_V is symmetrical about $\nu_{\rm O}$, the desired value for each line is twice the sum of these two quantities.

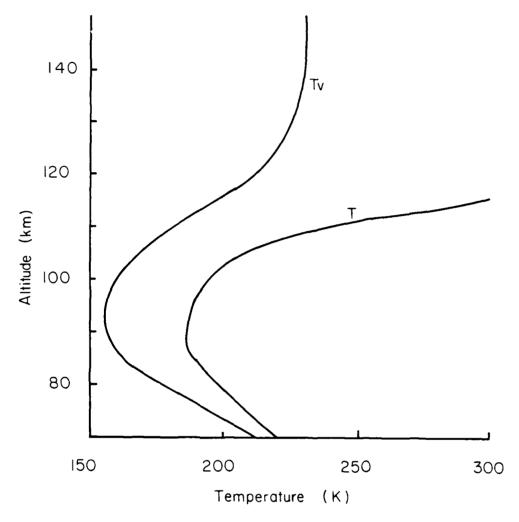


Figure 3. Kinetic and Vibrational Temperature Profiles Used to Calculate the Curves in Figure 2

The numerical integration procedure was designed to use the minimum number of integration points to obtain the desired accuracy. To accomodate the great variety of possible integrands, a semi-adaptive scheme is used. The region $\nu_{\rm O}$ to $\nu_{\rm C}$ is divided into sections, or panels, and the contribution to the total integral from each panel is evaluated separately using Gauss-Legendre quadrature. The panels are taken in order, starting at the line center with a fixed panel-width. At a certain point $\nu_{\rm B}$, beyond which the radiance profile is determined to be "smooth," the panels are allowed to increase in width so as to

cut down on the total number of integration points. The cutoff point $\nu_{\rm c}$ and the panel-expansion point $\nu_{\rm B}$ both depend on the radiance profile being considered, and they are determined as the integration progresses from panel to panel.

Each panel is integrated with the same fixed number of points. The default is four points, but two points per panel often give excellent results and of course require less computation.

The initial panel-width is one "standard Doppler width" (SDW). This is defined to be the half width at half maximum of a Doppler line with a frequency equal to that at the center of the band in question. The kinetic temperature used to define SDW is the lowest encountered in the atmospheric profile.

(1) Numerical Integration

The application of Gauss quadrature over panels of fixed width is a straight-forward exercise. In our case, once the integration has progressed into the smooth wing of the radiance profile--that is, past all extrema which might appear in I_{ν} --the panel widths are doubled in each successive panel. The condition used to establish that the function is smooth by this definition is that τ_{ν} be less than 0.5 at the end of the last panel previously considered. That is, $\nu_{\rm B}$ is chosen to be the end of the panel within which the path optical depth first drops below one-half.

The rationale behind this criterion for smoothness is that, for a fixed number of points, the absolute accuracy of any numerical integration algorithm is generally worst in intervals within which the integrand has maxima and minima. The validity of the corresponding choice for $\nu_{\rm B}$ is demonstrated in the following manner. One rewrites Eq. (14) as

$$I_{\nu}(s) = \langle R \rangle [1 - \exp(-\tau_{\nu}(s, s'))]$$
 (28)

by making use of the definition

$$\langle R \rangle = \int_{s'}^{s} R(s) F_{\nu}(s, s'') ds'' / \int_{s'}^{s} F_{\nu}(s, s'') ds''$$
 (29)

and the integrability of $F_{\nu}(s,s')$, as in Eq. (23), <R> is a function of ν . One sees that I $_{\nu}$ is the product of a weighted average of R and the absorptivity over the entire path. Bullitt et al show that <R> asymptotically approaches a limiting value, <R $>_{\infty}$, for large $|\nu - \nu_{_{\rm O}}|$, and that the departure from this limiting value is very modest whenever $\tau_{\nu}<$ 1. On the other hand, the absorptivity rapidly departs from its limiting value of unity only when $\tau_{\nu}>$ 1. Moreover, because of its functional form and because τ_{ν} decreases monotonically with

increasing ν , the absorptivity factor cannot by itself induce extrema in the radiance profile. One can then say that the functional form of the thick-line radiance profile dominated by <R> near the line-center and by the absorptivity in the wings, and that the extrema in I_{ν} must therefore be limited to the frequency range for which $\tau_{\nu} > 1$. To be conservative, we take $\tau_{\nu} \sim 0.5$ as the criterion for determining $\nu_{\rm B}$; in fact, we find that the outermost maxima in I_{ν} usually occur at frequencies for which $2 < \tau_{\nu} < 5$.

(2) Analytical Approximation After Cutoff

We cut off the numerical integration at $\nu_{\rm C}$ only when it has passed into the region $\tau_{\nu} <<$ 1. The contribution from this "tail" of the radiance profile is

$$T(\nu_{c}, s) = 2 \int_{\nu_{c}}^{\infty} I_{\nu}(s) d\nu$$
 (30)

From Eq. (11), this can be written as

$$T(\boldsymbol{\nu}_{c}, s) = \frac{A}{2\pi} \int_{s}^{s} n_{u}(s'') \left[\int_{\boldsymbol{\nu}_{c}}^{\infty} f_{\boldsymbol{\nu}}(s'') d\boldsymbol{\nu} \right] ds''.$$
 (31)

If the lineshape is a Voigt function, its functional form in the tail can be approximated by a Lorentz function, an asymptotic expansion of the Voigt integral, or some other means (see Section 2.3.5). One can then evaluate the ν -integral in Eq. (31), with the result that

$$T(\nu_{c}, s) = \frac{A}{2\pi^{2}} \frac{1}{\nu_{c} - \nu_{o}} \int_{s'}^{s} n_{u}(s'') \alpha_{L}(s'') ds''$$
(32)

where α_L is the Lorentz width due to the collision-broadening component of f_ν . In NLTE, of course, the integral is a sum over homogeneous layers. When this conversion is made and the Einstein absorption coefficient is used to replace A, with Eq. (10), the result is

$$T(\nu_{c}, s) = \frac{2}{\pi} \frac{1}{\nu_{c}, \nu_{o}} \sum_{i} \left[2c\nu_{o}^{2} \frac{g_{\ell}}{g_{u}} n_{u}(s_{i}) \right] \left[\frac{h\nu_{o}}{c} B_{\ell u} \right] \alpha_{L}(s_{i}) \Delta s_{i}$$
(33)

After substituting Eqs. (4) and (13) for the first quantity in square brackets and

Eqs. (17) and (18) for the second, most factors cancel, and one is left with a result expressed in simple terms:

$$T(\nu_{c}, s) = \frac{2}{\pi} \frac{1}{\nu_{c} - \nu_{o}} \sum_{i} R_{i} \alpha_{L}(s_{i}) \left[\frac{\Delta \tau_{\nu i}}{f_{\nu i}} \right]$$
(34)

In this equation, the term in square brackets and the other factors in the sum are independent of frequency [since, according to Eq. (18), the frequency-dependence of the optical depth is entirely contained in the lineshape]. The sum therefore needs to be evaluated only once for each line, say at ν_0 . It is then a simple matter, after the completion of the integration of each successive panel, to determine the approximate residual contribution from the entire region beyond that panel.

The more panels that are taken, the more accurate this residual term will be. The difficult part is determining just how accurate it is. Our procedure for determining $\nu_{\rm C}$, which is likely to be refined in the future, is based on empirical tests which show that if a quantity κ , defined as

$$\kappa = 6 \varepsilon I_{\rm c} / \tau_{\nu_{\rm c}} \tag{35}$$

is greater than $T(\nu_c, s)$, the fractional error introduced in I(s) by cutting off the numerical integration and adding T to the previous result will be less than ε . In Eq. (35), I_c is the cumulative integrated radiance in the panels treated so far, τ_{ν_c} is the optical depth for the path at the end of the last panel, and ε is the desired accuracy of the integrated radiance in the line, expressed as a fractional error. The optically thickest path is used to evaluate κ . This approximation is accurate enough to correctly evaluate the integral over a range contributing several percent to the total result in typical cases, and thus can eliminate numerical treatment of many panels in the far wing of the radiance profile.

If a Doppler, rather than Voigt, lineshape is selected, a different residual term is used in place of Eq. (34).

In order to evaluate Eq. (34), the collision-broadening linewidth $\alpha_L(s_i)$ must be computed for all relevant layers. For each line, the AFGL database contains a standard collision linewidth, α_o , calculated or measured for STP. This quantity is corrected for temperature and pressure to yield

$$\alpha_{L}(s_{i}) = \alpha_{o}P_{i}\left(\frac{T_{s}}{T_{i}}\right)^{X}$$
 (36)

where P_i and T_i are the pressure (in atmospheres) and the kinetic temperature in the ith layer, respectively. The exponent, x, to which the temperature ratio is raised, is equal to 0.50 for all molecules except CO_2 , for which a value of 0.75 is used.

2.3.4.2 Thin-Line Approximation

In the event that the path optical depth at the line center (and hence at all frequencies) is much less than unity, the integrated radiance can be computed analytically. In effect, one ignores absorption along the path and integrates the volume emission rate for the whole line along the path. If one takes Eq. (11) and sets the exponential equal to unity, only f_{ν} contains a ν -dependence. Upon inserting the result into Eq. (27), interchanging the order of integration, and using Eq. (5), one quickly arrives at

$$I(s) = \frac{A}{4\pi} \int_{s'}^{s} n_{u}(s'') ds''$$
(37)

After this integral is converted into a sum over homogeneous layers, one follows steps which are almost identical to those used to derive Eq. (34) from Eq. (32) to obtain

$$I(s) = \sum_{i} R_{i} \left[\frac{\Delta \tau_{\nu_{i}}}{f_{\nu_{i}}} \right]$$
(38)

This sum can be evaluated in a single loop through the atmosphere and therefore requires much less computational effort than the numerical integration.

The criterion that we use to determine whether Eq. (38) is an acceptable approximation to Eq. (27) is based on the value of the total path optical depth at the line center. For lines with

$$\tau_{\nu_0}(\mathbf{s},\mathbf{s}') < 3\varepsilon \tag{39}$$

NLTE bypasses the thick-line algorithm. ϵ is the quantity introduced below Eq. (35).

2.3.4.3 Accuracy

The NLTE algorithm has been designed to perform a detailed calculation and produce accurate results in a reasonable amount of computation time. The

accuracy of the calculation depends on the correctness of the input data, the physical approximations built into the algorithm, and the mathematical approximations used to implement it.

The greatest source of error in simulating a particular experiment will generally be due to uncertainties in the quantities contained in the atmospheric profile. For example, errors of a few degrees in a vibrational temperature profile can change the volume emission rate by significant amounts, especially for higher-energy transitions, with an ultimate effect that depends on the thickness of the lines in question and the altitudes at which the errors are most pronounced. Since one cannot anticipate the magnitude of errors of this sort, we focus on inaccuracies that could be induced by the algorithm.

(1) Layering Approximation

The principal physical approximation incorporated into this work is, of course, that of the homogeneous atmospheric layers. The magnitude of the errors induced depends on the (geometrical) thickness of the layers used, the gradients in temperature and number density, the degree of self-absorption along the path, and the path geometry itself. We estimate that with 1-km atmospheric layers, total errors in the integrated radiance will be less than 2 percent for any single line for most realistic atmospheric profiles. For bands containing both thick and thin lines, the error is likely to be much less than this. In both cases, the error will be in the direction of predicting too little radiance.

These conclusions are based on some hand calculations and also on the use of a contrived atmospheric profile. Since the number densities have a nonzero gradient at all altitudes and change by orders of magnitude over the range of the viewing paths, one's attention is first drawn to the approximation represented by Eq. (15b). Suppose that all number densities can be characterized by a local scale height everywhere -- that is, these functions are truly exponential within each layer. Then, assuming "correct" values $\rho(s_i)$ and $\rho(s_{i+1})$, Eq. (15b) gives the actual path-average number density only for zenith geometry. For limb geometry, greater distances are encountered in the lower part of each layer--particularly near the tangent point -- and this formula underestimates the path average by a small amount. As a result, both the optical depth and the volume emission rate are a little too small. From Eq. (11), one can see that, in general, these two errors tend to cancel, but the degree of cancellation depends on the optical depth. Intuitively, one suspects that the worst-case fractional error results for thin lines because the attenuation term, which in general compensates for the understated volume emission rate, is small.

To verify these conclusions, we used a contrived atmospheric configuration for which the correct path optical depth and the radiance, as well as the values that would be obtained by our algorithm, could be calculated analytically. The

assumptions were that of an equilibrium isothermal atmosphere, an exponential emitter density, and a Doppler lineshape. The correct integrated radiance for a single line under these conditions is

$$I(s) = R \int_{0}^{\infty} [1 - \exp(-\tau_{\nu}(s, s'))] d\nu$$
 (40)

and the two limiting values for I(s) are

$$I(s) \sim R \frac{\tau_{\nu_{o}}}{f_{\nu_{o}}} \qquad \qquad \tau_{\nu_{o}} << 1$$
 (41a)

$$I(s) \sim R \frac{\alpha_{D}}{\sqrt{\ln 2}} \sqrt{\ln \tau_{\nu_{o}}} \qquad \tau_{\nu_{o}} >> 1$$
 (41b)

where τ_{ν_0} is the path optical depth at the line center. Eq. (41b) results from an asymptotic expansion⁸ of the integrated absorptivity and is valid for the Doppler lineshape. The Doppler halfwidth, α_D , is given in Eq. (44) below.

With our simplifications, R is independent of altitude, and the NLTE result for I(s) is in error only because of the error in the optical depth. The value of the optical depth obtained by NLTE, $\overline{\tau}_{\nu_0}$, differs from the correct value by a small amount:

$$\overline{\tau}_{\nu_{\mathcal{O}}} = \tau_{\nu_{\mathcal{O}}} (1 - \delta) \tag{42}$$

The error term, δ , depends on the assumed scale height and is calculated analytically. Taking 1km for the layer thickness and 5km for the scale height, δ is 0.019 for limb geometry and 0.002 for zenith geometry; for an 8-km scale height, the values are 0.010 and 0.0007, respectively. From Eq. (41a), one can see that the worst-case single-line fractional error in I(s) is just δ and is associated with thin lines and limb geometry. For very thick lines, the fractional error is 1/2 δ / $\ln (\tau_{\nu_0})$ and is thus much smaller. Since most bands are dominated by the thick-line contributions, it follows that worst-case fractional errors in the band radiance

Van Trigt, C. (1968) Asymptotic expansions of the integrated absorptance for simple spectral lines and lines with hyperfine structure and isotope shifts, J. Opt. Soc. Am. 58:669.

due to the layering scheme are much less than δ , which is to say, for 1-km layers and typical atmospheric profiles, less than 1 percent.

These estimates, of course, ignore the effects of temperature gradients on the error induced by the layering approximation, but we believe that they are unimportant. Consider the approximation of the upper state vibrational temperature, T., by Eq. (15a). This quantity determines the volume emission rate and thus affects the radiance calculation. One can see that, in regions where T, has a sharp maximum Eq. (15a) understates it. (For limb-look, however, the path-average temperature is different from the layer-average, as before.) The error will be a factor of approximately exp ($c_2 E \Delta / T_v$), where E is the vibrational energy of the state and Δ is the error in T_v . A change in the vibrational temperature gradient equal to $0.5\,\mathrm{K/km}^2$, which is quite steep, gives a value of Δ on the order of $0.1\,\mathrm{K}$ for 1-km layers and 0.5 K for 2-km layers. For 1-km layers and a 2.7 μ m transition, the volume emission rate would err by, at worst, 1 percent in a few layers near the extremum. (For a lower-energy transition, the error would be much less.) In the very worst case, the extremum is a sharp maximum near the tangent point, and there is little attenuation at higher altitudes. In this case, the error adds to that discussed earlier; under most circumstances, however, it is considerably smaller, and the general estimates given earlier remain valid.

In extreme cases, inaccuracies due to the layering approximation can, of course, be reduced by using thinner layers, especially at the lowest levels.

(2) High-Altitude Cutoff

A second physical approximation is that all effects due to layers above a certain altitude can be ignored. For an arbitrary atmospheric profile and arbitrary line strengths, it is difficult to say, a priori, how many layers are needed. Generally, 50 1-km layers are adequate for bands dominated by thick lines.

One realization resulting from the tests we performed on NLTE is that, for lines quite far from the band center, the optical depth per layer may increase with increasing altitude, rather than the reverse, if the calculations extend into the lower thermosphere. This comes about because the elevated temperatures in the upper layers increase the lower rotational-state populations dramatically for such lines. This more than offsets the effect of decreasing total number density, and it means that many layers may be necessary if the precise contributions from such lines are needed. Because these lines are weak, their contribution to the radiance from a whole band is almost always negligible.

One can, of course, extend one's model atmosphere as high as is necessary to eliminate any possible error from this source.

(3) Overlap

The third physical approximation inherent in NLTE is that the lines are independent of each other--that is, that overlap is not a relevant consideration.

For the bands in the high-altitude non-LTE regions we usually consider, the lines are spaced sufficiently far apart--even in the Q branches--so that the numerical integration regions do not, in fact, run into each other. Since the numerical integration is cut off only when $\tau_{\nu} <<$ 1, as described in Section (2), the error induced by ignoring overlap is completely negligible for these cases. Of course, for very strong closely spaced lines and low-altitude viewing paths, overlap may be a relevant consideration. We have made no quantitative estimates of its effect on the integrated radiance, but it is clear that the error would be in the direction of predicting too much radiance.

(4) Mathematical Approximations

Several mathematical approximations employed in NLTE have been described earlier. They include use of numerical integration to evaluate Eq. (27) [(1) in Section 2.3.4.1], the thin-line approximation (Section 2.3.4.2), and the tail cutoff approximation [(2) in Section 2.3.4.1]. Also, the use of the Voigt function (Section 2.3.5) implies mathematical approximations as well as the physical assumption that that function is appropriate for the absorption cross-section. Last of all, approximations used to calculate the partition functions are discussed in Section 2.3.7.

In the case of the numerical integration, one can only check the accuracy by comparing results using different numbers of integration points per panel. In all cases we have tested, the difference between using four points and using eight points is on the order of 0.01 percent or less, and thus negligible.

Two other approximations are scaled to the nominal desired accuracy, ε , and thus can be made as small as necessary. The thin-line approximation produces a worst-case fractional error of almost exactly ε . That is, if the line falls just below the thin-line threshold, the error is ε times the computed intensity and is positive (too much radiance). Weaker lines produce smaller errors, so using the default value ε = 0.01, the error induced in the integrated band radiance by this approximation alone will be less than 1 percent even if there are few contributions from thick lines to be added in.

In a single-line run, NLTE ignores the thin-line criterion and calculates the radiance numerically even for very weak lines.

Similar considerations apply to the analytical tail approximation. The worst-case error for a single line is approximately ϵ , but the average error is considerably less, and the resultant effect on the band radiance is thus quite small.

The Voigt algorithm is discussed in the next section. It is so accurate that it does not contribute to the error in I(s). The partition function approximations also contribute a negligible amount to the final error.

(5) Summary

The algorithm has been refined to the point where the uncertainties in the atmospheric profile used as input must be regarded as the dominant source of

error in the integrated radiance calculated by NLTE. The only exceptions to this would come if a very coarse altitude grid were used, or possibly if extremely disturbed atmospheric conditions (for which we have not checked our approximations) were assumed.

2.3.5 VOIGT ALGORITHM

It is very important to account for collision-broadening in the absorption cross section, even in high-altitude regions where collisions are relatively infrequent and the ratio of the collision linewidth to the Doppler linewidth is very small. This is true because many lines may be severely self-absorbed in the line center even for paths traversing only very high-altitude regions. In such cases, the contribution in the wings, where the collision component dominates, constitutes a large part of the total radiance profile. It is, therefore, necessary to have an accurate representation of the lineshape in the wings, which is to say that the Voigt rather than Doppler profile must be used. Errors of 50 percent to 100 percent can easily be made by neglecting collision-broadening.

The Voigt function, which is the convolution of a Lorentz function and a Gaussian, can be specified by two parameters: the linewidth ratio, y, and the normalized frequency, x:

$$y = \sqrt{\ln 2} \frac{\alpha_{L}}{\alpha_{D}}$$
 (43a)

$$x = \sqrt{\ln 2} \frac{\nu - \nu_{o}}{\alpha_{D}}$$
 (43b)

 $\alpha_{\rm L}$ and $\alpha_{\rm D}$ are the collision-broadened and Doppler linewidths, respectively, and are functions of altitude. $\alpha_{\rm L}$ is given in Eq. (36) and $\alpha_{\rm D}$ is

$$\alpha_{D} = \nu_{O} \left(\frac{2 \ln 2 kT}{Mc^{2}} \right)^{1/2}$$
(44)

where M is the mass of the molecule, k is Boltzmann's constant, and c is the speed of light.

We originally used a very accurate Voigt routine due to Rybicki⁹ (VWERF),

^{9.} A method due to Rybicki, described in Emission, Absorption, and Transfer of Radiation in Heated Atmospheres (1972), B.H. Armstrong and R.W. Nichols, Pergamon, New York.

which correctly gives eight significant figures over the entire x-y plane. An algorithm due to Pierluissi et al 10 (ZVOIGT, which pieces together three formulas to cover the plane) runs considerably faster but is inaccurate in the near wings (x \sim 3) for an important range of values of y. To speed our calculations, we rewrote Pierluissi's algorithm so that it gives results which are accurate to at least 0.1 percent in the line center (x < 1.25) and 0.5 percent everywhere else except where y < 10^{-6} . To accomplish this, we checked the accuracy and speed of routines using different representations of the Voigt function throughout the x-y plane. We then pieced them together in such a way that the fastest routines occupy as much of the plane as possible, and the calls to the routines and the logical branches to the different regions use as little compute time as possible. A detailed description of our routine, ZVGTC, will be given elsewhere; in this section, we mentioned only a few points which are relevant for NLTE.

In the previous paragraph, we indicated the minimum accuracy criterion for ZVGTC. In fact, it is only near the boundaries between regions where these limits are approached. Over much of the plane, especially in the line center with y>0.001, its accuracy is six figures or better. We have tested NLTE with both VWERF and ZVGTC and have found no differences in the final results for the radiance. The advantage of ZVGTC is that it runs in less than one third of the time required by VWERF.

Figure 4 shows the division of the x-y plane into the four regions used in ZVGTC. Region 1 is treated using Pierluissi's series expansion 10 modified to deal with an extended range in x. Regions 2 and 3 use 6- and 2-point Gauss-Hermite quadrature, respectively. 11 These formulas involve only rational functions and are very fast. For thick lines, a large fraction of the function evaluations fall in these regions. In Region 4, we substitute the Dopple profile for the actual Voigt function, in the interest of speed.

The arithmetic used for Regions 2-4 is fast enough so that branching operations encountered in the subroutine actually begin to compete with the function evaluations for computation time. The peculiar shape of Region I results from a need to avoid transcendental function evaluations in the branches. For similar reasons, we avoid repeated entries to the routine by evaluating the Voigt function for many

Pierluissi, J.H., Vanderwood, P.C., and Gomez, R.B. (1974) Fast calculational algorithm for the Voigt profile, <u>J. Quant. Spectrosc. and Rad. Transfer 18:555.</u>

^{11.} Kalshoven, J.E., Jr., and Walden, H. (1983) Laser bandwidth and frequency stability effects on remote sensing of atmospheric pressure as applied to a horizontal path measurement, paper presented at topical meeting on Optical Techniques for Remote Probing of the Atmosphere, Incline Village, Nev.

layers all at once, using a loop within the subroutine rather than one in the main program.

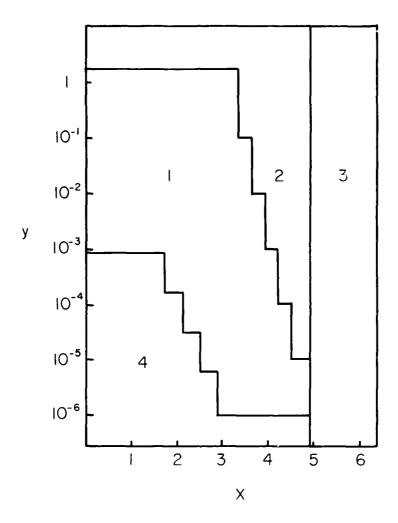


Figure 4. Segments of the x-y Plane Allocated by the Voigt Routine ZVGTC. In Region 1, the Voigt 'unction is evaluated using the ZVOIGT series. ¹⁰ In Regions 2 and 3, 6- and 2-point Gauss-Hermite quadrature are used, respectively. In Region 4, the Doppler profile is substituted

2.3.6 SYNTHETIC SPECTRUM

To simulate the imperfect resolution of a real detector, NLTE evaluates a simple sum that approximates the convolution of the calculated spectral radiance with an instrumental scanning function.

In general, if I_j ($\nu - \nu_0$) represents the radiance profile of the jth line at wavenumber ν , and $g(\nu - \nu')$ is the scanning function—the pattern through which the intensity at ν' is redistributed to ν by the instrument—the contribution to the observed spectrum due to this line is

$$G_{j}(\nu) = \int I_{j}(\nu' - \nu_{o}) g(\nu - \nu') d\nu'$$
 (45)

g must be normalized to unity. Observe that our notation is slightly altered: The quantity in the integrand is what we previously called $I_{\nu}(s)$.

In NLTE, calculation of this synthetic spectrum is simplified by two assumptions. First, we take the instrument function to be triangular in shape:

$$g(\nu - \nu_{O}) = [\Delta - |\nu - \nu_{O}|]/\Delta^{2} \qquad |\nu - \nu_{O}| \leq \Delta$$
 (46a)

$$g(\nu - \nu_0) = 0 \qquad |\nu - \nu_0| > \Delta \qquad (46b)$$

where Δ is, by definition, the full width at half maximum of the function. Second, we assume that g is much broader than the width of the individual-line radiance profiles, and that the latter may therefore be approximated by delta functions:

$$I_{j} \left(\nu - \nu_{o} \right) \sim I_{j} \delta \left(\nu - \nu_{o} \right) \tag{47}$$

where \mathbf{I}_j is the integrated radiance determined by NLTE. The convolution is then trivial, and the spectral radiance is given by a sum over lines:

$$G(\nu) = \sum_{j} G_{j}(\nu) = \sum_{j} I_{j} \frac{\Delta - |\nu - \nu_{oj}|}{\Delta^{2}}$$
 (48)

By requiring the intensity to be "located" at each line's center, this procedure, of course, obscures any details of the individual radiance profiles.

2.3.7 PARTITION FUNCTIONS

In order to calculate the optical depth in the various layers via Eqs. (18) and (19), one uses the vibrational and rotational partition functions, Q_{V} and Q_{R} . It happens that these appear only in ratios: the partition function for conditions pertinent to a particular layer divided by the partition function for LTE conditions at the standard temperature, T_{S} .

We take the vibrational partition function to be similar to the harmonic-oscillator partition function.

$$Q_v(T_v) \sim [1 - \exp(-c_2 E_o/T_v)]^{-D}$$
 (49)

where $\rm E_{_{O}}$ is the energy of the oscillator fundamental, $\rm T_{_{V}}$ is the vibrational temperature, and D is the degeneracy of the excited states. For diatomic molecules, this is an approximation in that it assumes equally spaced levels and a single vibrational temperature giving the populations of all the states. For triatomic molecules, we assume that $\rm E_{_{O}}$ refers to the lowest-lying ladder of states, and thus make the additional approximation of not counting the states in the other ladders. (For example, in $\rm CO_2$ we take $\rm E_{_{O}}$ = 667.379 cm⁻¹ and D=2, corresponding to the ν_2 fundamental, and thereby neglect the ν_1 states, the ν_3 states, and the combination states. A better approximation in this case would be to use the product of three such functions, but this still neglects the combination states.

In fact, these approximations are excellent ones. At normal temperatures, neglect of the ν_1 and ν_3 states reduces Q_v by about 0.1 percent and 0.002 percent, respectively, for CO2. The differences due to anharmonicity are similarly small. The fact that Q_v appears as a ratio further dilutes the effect of these errors. The uncertainties associated with any vibrational temperature profile clearly dominate the errors caused by these approximations.

For $\mathrm{CH_4}$, the energy levels are more complicated, but $\mathrm{Q_V}$ can be approximated to about 1 percent ¹² by taking empirical values of 1370 cm⁻¹ and 5 for $\mathrm{E_O}$ and D, respectively.

For O_2 , several transitions in the near infrared are electronic transitions, but NLTE treats them as if they were vibrational transitions. In this case, Eq. (49) is, of course, wrong in principal. The levels are so high-lying, however, that O_v is practically identical to unity, and, in practice, Eq. (49) is perfectly adequate.

^{12.} Bullitt, M.K. Private Communication.

The temperature dependence of the rotational partition function is approximated by

$$\frac{Q_R(T)}{Q_R(T_s)} = \left(\frac{T}{T_s}\right)^j \tag{50}$$

where the exponent, j, is unity for linear molecules, and 1.5 for nonlinear molecules. $^{2}\,$

3. USE OF THE PROGRAM

3.1 Introduction

NLTE is written in FORTRAN'77. It requires about 106000 (decimal) words to compile and load on the CYBER 750 at AFGL. A high-optimization option should be selected at compile time (OPT=2 on the FTN5 compiler) if a full band is being run. Each run requires about 2 seconds to perform all the initialization steps, and then a fraction of a second for each line considered. The exact amount of time required, of course, depends on the amount of computation to be done-that is, on the optical depth of the line, the number of atmospheric layers, the number of integration points selected, and so on--but it is typically about 0.25 sec. per line on the CYBER.

NLTE requires information from three data files, which are associated with units 1, 2, and 3. These files contain general program directives, an atmospheric profile, and a coded AFGL line file, respectively. We reiterate that program NLTE, in its stand-alone form, deals with single vibrational bands. As such, the program input on units 1 and 2 is specific to the band in question. (In fact, unit 1 identifies the band.) To obtain the total radiance from several overlapping bands, it is necessary to run the program several times. On unit 3, data pertaining to bands other than the one of interest are ignored.

NLTE prints output on units 4, 5, and 6, with unit 4 being used for the principal results and units 5 and 6 containing supplementary and diagnostic information. If a synthetic spectrum is calculated—that is, if an instrumental scanning function is specified (see Section 2.3.6), NLTE writes the spectral radiance to unit 7 as well as to unit 4. To obtain the total spectral radiance of overlapping bands, the program must be run once for each band. On the first run, a new file is associated with unit ; on succeeding runs, the earlier file is read, the results for the new bands are added in, and the same file is rewritten so that the cumulative results are available. This is all done automatically, provided that the original

file is available and the instrumental scanning function and certain other parameters are the same.

The present version of NLTE is written so that an optional file associated with unit 9 can be created for use in interactive mode. This feature is discussed in Section 3.3.5.

On the CYBER 750, the default filenames TAPE1-TAPE6 are used for the files associated with units 1-6. Unit 7, if selected, is associated with file SPECF. Unit 9 is associated with OUTPUT on the CYBER.

Units 2 and 3 are rewound before they are read; unit 1 is not. One can thus put program directives for several runs on (separate records of) unit 1 if the runs are to be done consecutively. Unit 7, if it is used, is also rewound before it is read. Except for unit 9, all files to which NLTE writes output are rewound before normal termination of the program.

Appendix C contains the source listing for NLTE. Appendixes A and B give sample program input and output for two separate jobs--one which calculates the radiance from an entire band, and another which gives the results for a single ro-vibrational transition. They also contain the command sequences used to run these jobs on the CYBER.

3.2 Input Requirements

Unit 1 contains general program directives; nd physical parameters describing the transition(s) being considered. It is read with list-directed reads, which allows for flexible input formatting and makes it easy to use defaults. In fact, many of the quantities, particularly the program directives, have built-in defaults which do not need to be changed by the user in most circumstances.

Units 2 and 3 are each read in fixed formats, described below. In general, there are no default values for the quantities read from these files; however, on unit 2, the program will, as discussed in Section 3.2.2.3, interpret the input fields in a way which varies with the circumstances.

All three input files may begin with header cards containing alphanumeric information to identify their contents. Header cards are identified by the character C in the first column. Any number of header cards may be included at the beginning of the files, but after the first actual data are read, all information is interpreted as data. That is, "comment cards" cannot appear in the bodies of the input files.

Sections 3.2.1-3.2.3, below, describe the input information for the three required data files.

3. 2. 1 UNIT 1: GENERAL PROGRAM DIRECTIVES

Table 1 lists the program input obtained from unit 1. The list-directed read allocates one field, of arbitrary length and delimited by commas or blanks, for each variable. Variables corresponding to null fields—defined, for example, by consecutive commas—are unchanged from their previously-set default values. A slash (/) after any field terminates the read operation and defines the remaining fields as nulls. It is thus necessary to provide numerical or character input only for those quantities for which no default is listed in Table 1. For list-directed reads, all character variables must be enclosed in single quotes (!), as indicated.

Appendixes A.1 and B.1 contain sample input for two different jobs. Sections 3.2.1.1 - 3.2.1.5, below, discuss the information read from the four or five card-images comprising file TAPE1.

3.2.1.1 1A: Line Directives

Information on the line directives card identifies the transitions under consideration. The molecule code is a character variable corresponding to one of the first eight infrared-active molecule, included in the AFGL database—that is, 'H2O', 'CO2', 'O3', 'N2O', 'CO', 'CH4', 'O2', or 'NO' should be read. The isotope code and the designation of the vibrational states are standard AFGL notation. For linear molecules only, within the band identified by UST and LST, one may consider only the P, Q, or R branches, or else all branches (default). For the branch(es) considered, one may choose a single rotational quantum line—identified by NRL, the J quantum number of the lower rotational state—or all the lines (default).

3.2.1.2 1B: Viewing Path Parameters

The viewing path parameters define the line-of-sight of the observer. NLTE can handle limb- or zenith-look geometry. In limb-look, the path is parameterized by a single quantity, the tangent height. The observer is presumed to be above the atmosphere and the path extends from space to space through the tangent point. In zenith-look, the sensor looks directly upwards from some point within the atmosphere. The path is parameterized by this observation height.

NLTE is capable of calculating the radiance over many-but not more than 50 --viewing paths in a single run. The viewing path parameters are defined by a range (TANI-TANF) and spacing interval (SPAC) rather than a set of discrete values. Limb- and zenith-look geometry are distinguished by the sign of SPAC. If SPAC is positive, NLTE assumes limb-look; if SPAC is negative, NLTE computes the radiance in the zenith. For example, if card 1B contains "70, 85, -5", observation heights of 70, 75, 80, and 85 km are assumed for the zenith calculation. If a band-radiance calculation involves more than 500 lines, only five viewing paths can be run at once.

Table 1. Program Input on Unit 1

Variable De	scription	Units	Type	Example	Default
CARD 1A:	Line Directives				
MOL	Molecule code		Char	'CO2'	_
ISO	Isotope code		Integer	626	_
UST	Upper vib level		Char	'01101'	_
LST	Lower vib level		Char	'00001'	_
BR	Branch (P, Q, R, A)		Char	'ହ'	'A'
NRL	Rot'l Line number		Integer	14	999
CARD 1B:	Viewing Paths				
TANI	Lowest tang or observ ht	km	Real	70	_
TANF	Highest tang or observ ht	km	Real	85	TANI
SPAC	Interval	km	Real	5	+1
CARD 1C:	Program Directives				
HMAX	Top of atmosphere	km	Real	130	see text
ACC	Accuracy	_	Real	0.05	0.01
NPTS	Integ pts per panel	_	Integer	2	4
NDP	Lineshape code		Integer	0	0
VMIN	Low end, freq range	cm ⁻¹	Real	600	0
VMAX	High end, freq range	cm ⁻¹	Real	800	20,000
CARD 1D: S	Synthetic Spectrum Parameters				
FWHM	Width of scanning fn	cm^{-1} , μm	Real	20.1	0
DEL	Spacing of points	cm^{-1} , μm	Real	2	1
UNIT	Units of FWHM and DEL	-	Char	'CM-1'	'CM-1'
CARD 1E: 1	Band parameters**	***************************************		· · · · · · · · · · · · · · · · · · ·	
VIBE	Vib energy of transition	cm ⁻¹	Peal	667.379	
VIBL	Vib energy of lower state	cm ⁻¹	Real	0.0	_
VIBQ	Vib quantum in part'n fn	cm^{-1}	Peal	667.379	
GL	Statistical wgt, lower st	_	Integer	1	_
GU	Statistical wgt, upper st	_	Integer	2	_
**Note that	card 1E is sometimes superfluor	ıs (see text)			 , , ,

3.2.1.3 1C: Program Parameters

HMAX is the highest altitude to be considered in performing the calculation-that is, the "top" of the atmosphere. It should be sufficiently greater than TANF so that the radiance contributions from higher (neglected) altitudes are of little consequence. It defaults to the highest altitude in the profile read on unit 2.

ACC is the nominal accuracy of the integrated radiance computed for each individual line, expressed as a fractional error. It was introduced as ε in Section 2.3.4. Except for the numerical integration, all the mathematical (as opposed to physical) approximations are designed to contribute errors in the end results which are smaller than this amount.

NPTS is the number of integration points per panel in the numerical integration over frequency. Acceptable values are 2, 4, and 8. We know of no way to assess the accuracy of the integration procedure except to increase this parameter. However, for most cases we tested, using the default value (4) instead of the maximum value (8) introduces errors of less than those allowed by specifying ACC = 0.001.

The lineshape code, NDP, can have the values -1, 0, and 1. The default value, 0, selects the new Voigt routine ZVGTC. A value of +1 gives the Doppler lineshape. A value of -1 accesses Voigt function VWERF, which is very accurate but much slower than ZVGTC. We have not found any case in which the older routine gives significantly different results.

VMIN and VMAX define the range of line positions to be searched on unit 3 for transitions to be considered. Default is to search the entire file.

3.2.1.4 1D: Synthetic Spectrum Parameters

If a synthetic spectrum is desired, a positive number must be read for FWHM; otherwise the default condition (no synthetic spectrum) is assumed. The result is in units of watt/(cm²-ster-cm⁻¹) or watt/(cm²-ster- μ m), depending on UNIT. Possible values of UNIT are 'CM-1' and 'UM'. If spectra from previous runs are being added in, FWHM, DEL, and UNIT, as well as TANI, TANF, and SPAC, must all be exactly the same as the earliest values. No more than 12 synthetic spectra will be generated, even if the number of viewing paths is greater.

3.2.1.5 1E: Band Parameters

In order to perform the radiance calculation, NLTE uses five parameters which represent properties of the vibrational 1c/els under consideration. In order to ease the input requirements, these properties of many important levels of two important molecules. CO_2 and NO, have been stored in BLOCK DATA MOLPAR for automatic retrieval by the program. For other molecules and for CO_2 and NO levels not included in this database, however, it is necessary to read in these

quantities. The fifth data card must then be included on unit 1.

The three energies needed are VIBE, the energy of the vibrational transition, which is needed to calculate γ ; VIBL, the vibrational energy of the lower state, needed for P_{ℓ} and also for other purposes; and VIBQ, the energy of the lowest lying vibrational state, needed to calculate the vibrational partition function. The statistical weights of the upper and lower states are used to calculate the populations of the vibrational levels. Table 2 gives the list of vibrational levels for which the necessary information is stored. Card 1E can be omitted if the radiative transition connects any two of these vibrational states.

3.2.2 UNIT 2: ATMOSPHERIC PROFILE

3.2.2.1 Requirements for the Atmospheric Profile

The information contained on unit 2 defines the model atmosphere. Since NLTE provides no means of determining the populations of the radiating states independently, it is necessary to read a sufficient amount of data to enable such a calculation for all altitudes of interest. The information read pertains to vibrational levels, not ro-vibrational levels. (The ro-vibrational populations are derived using a rotational temperature equal to the kinetic temperature). The vibrational partition function, $Q_{\rm V}$, is also needed and information used to evaluate it is contained on unit 2.

We distinguish between regular bands, in which the lower vibrational state is the ground vibrational state, and hot bands in which the lower vibrational state is not ground. In general, we regard each vibrational state as having its own vibrational temperature, even though, in practice, strongly-coupled levels may be described by the same temperature profile. Because the vibrational temperature of the ground state is not meaningful, less input information is required for regular bands than for hot bands.

Since the vibrational levels may be described in alternate but equivalent ways, NLTE provides different input options for users with model atmospheres expressed in terms of different quantities. For regular bands, the populations of the upper and lower radiating vibrational states may be calculated from the total number density and the upper-state vibrational temperature, or conversely. For hot bands, the total number density is required, but one may specify either the number densities or the vibrational temperatures of the upper and lower radiating vibrational states. NLTE allows for input in various combinations, and it distinguishes them automatically according to criteria discussed in Section 3.2.2.3.

For the partition function, the approximation discussed in Section 2.3.7 requires the vibrational temperature of the lowest vibrational level of the molecule. This can be read directly or calculated from the number density of this

Table 2. CO2 and NO Vibrational Levels Included in MOLPAR

		CO	2 leve	els				N	O lev	/els	
iso	626	636	628	627	6 3 8	637	828		46	56	48
level								level			
00001	x	x	x	x	x	x	x	0	x	x	x
01101	x	x	x	x	x	x	x	1	x	x	x
10002	x	x	x	x	x	x	x	2	x	x	х
02201	x	x	x	x	x	x	x	3	x		
10001	x	x	x	x	x	x	x	4	x		
11102	x	x	x	x				5	x		
03301	x	x	x	x				6	x		
11101	x	x	x	x							
00011	x	x	x	x	x	x	x				
20003	x	x	x	x							
12202	x	x	x	x							
20002	x	x	x	x							
04401	x	x	x	x							
12201	x	x	х	x							
20001	x	x	x	x							
01111	x	x	x	x							
10012	x	x	x	x							
02211	x	x	x	x				Ì			
10011	x	x	x	x				l			
11112	x	x	x	x							
03311	x	x	x								
11111	x	x	x	x							
00021	x	x	x	x							,
20013	x	x	x	x							į
12212	x	x	x								
04411	x	x	x								
20012	x	x	x	x							
12211	x	×	x								
20011	x	x	x	x							

level and that of the ground state. NLTE automatically distinguishes between these two possibilities, also.

3.2.2.2 Input Format

Unit 2 is read using a formatted read which is the same for all options. Following the header, the card-images each contain all the information pertaining to a single altitude. They are ordered according to increasing altitude. No more than 250 altitudes, corresponding to 249 layers, can be read. The format is (F5.1, F10,3, 5E12.5, A15), where the first two fields are reserved for the altitude and temperature, and the next five are for the various allowed combinations of number densities and vibrational temperatures. The character field is used for overriding the default interpretations of the input data. (See Sections 3.2.2.3 and 3.2.2.4.)

The variables which can be read from unit 2 are defined in Table 3. The last three variables are used only for approximating the partition function. There are 11 options for reading the data, each involving a different combination of these quantities. Six options pertain to regular bands, four to hot bands, and the last implies LTE conditions and is therefore useful for both regular and hot bands. The combinations are listed in Table 4.

Table 3. Variables Read from Unit 2

* ALT ----the altitude (km) (required)

* TRTMP-- the translational temperature (K) (required)

* RHO -----the total number density (molecules/cm³). This includes all isotopes.

* TVL -----vibrational temperature of the lower level (K). (Hot bands only.)

* TVU -----vibrational temperature of the upper level (K)

* NL------number density of the lower vibrational level (molecules/cm³).

Unlike RHO, this refers only to the isotope under consideration.

* NU------like NL, but for the upper vibrational level

* TVQ -----vibrational temperature of lowest excited state (K)

* NO------number density of the ground vibrational state (molecules/cm³), for the isotope under consideration

* N1------like NO, but for the lowest excited vibrational state

Appendixes A.2 and B.2 contain sample atmospheric profiles using two different input options. A.2 illustrates the use of vibrational temperatures on input (option 7). B.2 illustrates the use of number densities for both the radiative transition and the vibrational partition function.

Table 4. Possible Combinations of Input Data on Unit 2.

Option

Regular Bands:

- 1. ALT, TRTMP, RHO, TVU, TVQ
- 2. ALT, TRTMP.RHO, TVU, NO, N1
- 3. ALT, TRTMP, NL, NU, TVQ
- 4. ALT, TRTMP, NL, NU, NO, N1
- 5. ALT, TRTMP, RHO, TVU
- 6. ALT, TRTMP, NL, NU

Hot Bands:

- 7. ALT, TRTMP, RHO, TVL, TVU, TVQ
- 8. ALT, TRTMP, RHO, TVL, TVU, NO, N1
- 9. ALT, TRTMP, RHO, NL, NU, TVQ
- 10. ALT, TRTMP, RHO, NL, NU, NO, N1

LTE Conditions:

11. ALT, TRTMP, RHO

With options 1-4, a redundancy is implied if the radiative transition connects the ground and first excited states because, for example, TVU and TVQ are identical. In this case, option 5 or 6 can be used. If, on the other hand, the radiative transition connects a higher state, use of option 5 will require that the vibrational partition function be calculated with the vibrational temperature appropiate for the radiating states rather than that for the lowest lying levels. This leads to errors in the radiance calculation which will be quite small for most quiescent conditions. For option 6, the radiance will be correct, although quantities which are printed but not used will be slightly in error.

For options 7 and 8, a blank field, or zero, in place of TVU will cause the program to equate TVL and TVU--that is, use the same profile for both

vibrational temperatures.

3.2.2.3 Default Interpretations

NLTE automatically distinguishes among the 11 allowed combinations. It does so by interpreting the data on the first card-image--that is, the data describing the lowest altitude included on the file--according to the numerical values appearing in special fields. These special fields are the fourth and fifth fields for regular bands, and the fourth and sixth fields for hot bands. The numbers in them can either be zero (blank fields) or can represent a vibrational temperature or a number density.

Vibrational temperatures generally have numerical values between 100 and 500, while number densities are usually much larger. The default criteria for distinguishing among options are: (1) A nonpositive numerical value in a special field indicates unavailable data; (2) A positive value below 1000 indicates a vibrational temperature; (3) A value above 1000 indicates a number density. For regular bands, for example, reference to Table 4 shows that options 1 and 3 differ from options 2 and 4 because the partition function may be calculated directly from TVQ or indirectly from NO and N1. The value of the quantity appearing in the fifth data field identifies it as either NO or TVQ, and the range of possibilities is narrowed accordingly. Similarly, the quantity in the fourth field is either NU or TVU. Its value distinguishes between options 1 and 3 or between options 2 and 4. A blank in field 5 implies option 5 or 6. A blank in field 4 implies option 11: no vibrational temperatures are available, so the translational temperature is used to calculate all populations.

3.2.2.4 Override Code

NLTE provides an override capability for the default interpretations, to allow for possible ambiguities. For example, data intended to be read with an option 9 interpretation might be mistakenly read with option 7 if the upper radiating state is only populated to the extent of a few hundred molecules/cm³. In that case it would be necessary to read a character variable, CODE (only on the lowest-altitude card-image), to orient the program properly.

CODE should appear as three consecutive characters anywhere in columns 76-90 of the lowest altitude data card. It should not be delimited with quotes. Table 5 gives the proper override codes and the options which they force into effect.

Table 5. Override Codes

CODE	Action
	default interpretation
LTE	LTE conditions prevail
т, т	requires option 1 or 7
T, N	requires option 2 or 8
N, T	requires option 3 or 9
N, N	requires option 4 or 10

3.2.3 UNIT 3: LINEFILE

3.2.3.1 Requirements for the Linefile

The properties of the lines used in the radiance calculation are taken from unit 3. This is a coded linefile, a subset of the AFGL Atmospheric Absorption Line Parameters Compilation², ³, ⁴ maintained by personnel at AFGL/OPI. The quantities read by NLTE are given in Table 6, as is the format determined by the larger database.

Table 6. Line-File Data for Each Ro-Vibrational Transition

Format	Symbol	Line-file Datum
F10, 4	ν_{\circ}	Resonant Frequency (cm ⁻¹)
E10.3	S(T _s)	Line Intensity (LTE, 296K) (cm ⁻¹ /mo1-cm ²)
F5.4	αο	Lorentz half-width (1 atm) (cm ⁻¹ /atm)
F10.3	E''	Energy of the lower state (cm $^{-1}$)
2A8, A10, A9		Quantum numbers, line identifiers
13		Entry code for these data
14	ISO	Isotope code
13	MOL	Molecule code

The physical data in Table 6 have been discussed earlier. The total lower-state energy, E", is needed to obtain the rotational energy, E_R " for the calculation of Eq. (19). The entry code and the molecule code are not checked by NLTE. The isotope code is the same as the variable ISO read from unit 1. The quantum numbers and line identifiers are different for different molecules. 2 In fact, the corresponding formats are different as well. NLTE reads each file in a format appropriate for the molecule being considered.

Appendices A.3 and B.3 give examples of coded linefiles appropriate for input to NLTE .

3.2.3.2 Obtaining the Linefile

The AFGL Atmospheric Absorption Line Parameters Compilations has been described in many publications, 2 , 3 , 4 At AFGL, it resides on a disk pack to which it was written in buffered binary form. Dr. L.S. Rothman, who is responsible for the compilation, has prepared a Cyber Control Language procedure, WRITE, for obtaining coded subsets of the database.

Users who do not have access to Dr. Rothman's disk pack can obtain the linefile information from magnetic tape. The data format and a possible approach to acquiring files from this medium have been discussed in the report 1 accompanying the first release of NLTE, and we refer readers to that publication for this information.

Example 1 gives a control-card sequence which obtains, saves, and lists all ozone lines between 2000 and 2020 cm⁻¹ using WRITE. The GET command locates the file containing the procedure and the BEGIN command invokes it. The latter contains optional parameters, described in Table 7, which determine the disposition of the information acquired from the compilation. The data card(s) following the end-of-record provide the information the procedure requires to identify the desired lines.

EXAMPLE 1 Use of the Procedure WRITE

```
JOB. . .

USER. . .

CHARGE. . .

GET, P = PROCEDU/UN=ROTHMAN.

BEGIN, WRITE, P, PFN=OZONELN, COPFIL=YES.

---EOR--

2000, 2020, 'O3', , , , 'PFILE'
```

(1) Identifying the Lines

The information to be taken from the data cards is listed in Table 8. Each card is read with a list-directed read, which means that the data fields (eight in

Table 7. Parameters for the Procedure, WRITE

KEYWORD	VALUE	DEFAULT
PFN	Permanent File Name	No save is done even if PFILE is specified on some data cards
COPFIL	YES	NO (no list of TAPE8)
SORTM	YES	NO (no SORT/MERGE)

number) should be separated by comma delimeters and no attention need be paid to the columns used for each field. Default values result from blank fields (consecutive commas). After the last field containing a nondefault value, a slash (/) can be used to terminate data input for that card. Either the slash or a sufficient number of commas to define each field must be used. All input data of type character must be surrounded by single quotes. Leading blanks inside the quotes will give unpredictable results. Anywhere else, blanks are irrelevant. Any number of cards can be included.

Table 8. Input Data for the Procedure, WRITE

DATUM	QUANTITY	TYPE	DEFAULT
V1, V2	Frequency Range (cm ⁻¹)	Integer, Real	None
MOL	Molecular Formula	Character	All molecules
ISO	Isotope Code	Integer	All isotopes
UST, LST	Band quantum numbers	Character	All bands
SCRIT	Threshold Strength	Real	All strengths
DISPOS	File Disposition Code	Character	List only

V1 and V2 must be specified, as there is no default. MOL is the alphanumeric symbol giving the molecular formula. ISO is the isotope code. UST and LST are the upper- and lower-state quantum numbers for the vibrational bands desired. The quantum numbers are different for different molecules, and their meaning is discussed by McClatchey et al. Por the purposes of WRITE, one enters consecutive digits inside quotes, for example, '11101.'

SCRIT is the intensity threshold. Lines which are weaker than this threshold are ignored. Because of the small magnitudes involved, an E descriptor should be used.

The data selected by the procedure can be either listed on OUTPUT or written to TAPE8, which is defined as a direct-access permanent file. DISPOS is a code used to select the desired disposition. Entering 'PFILE' in this field causes TAPE8 to be written. Anything else invokes the list option. One can list some data and save other data by entering different disposition codes on different cards.

Lines satisfying the requirements of each separate data card are frequency-ordered on whichever file they are directed to. However, lines from one data card will always follow those from preceding cards. If the frequency ranges are increasing and do not overlap, frequency-ordering is preserved. Otherwise, for TAPE8, only, a SORT/MERGE option can be specified on the BEGIN card to restore frequency-ordering. Frequency-ordering is not necessary for NLTE.

(2) Parameters for WRITE

The BEGIN card invokes the procedure WRITE (which is found on logical file P in our example). It allows up to three optional parameters which are used for separate purposes: to preserve the frequency-ordering on TAPE 8, as mentioned above; to give the permanent file name; and to cause the information on TAPE8 to be copied to OUTPUT. The form of each of these parameters is KEYWORD=VALUE where KEYWORD is fixed and VALUE is supplied by the user. Table 7 describes these parameters. The parameters can be entered in any order following the logical file name. Parameters which are omitted assume default values, the effect of which is given in Table 7.

3.3 Program Output

Appendixes A. 4-A. 7 and B. 4-B. 6 contain program output for Sample Runs 1 and 2. In general, each of the output files (units 4, 5, and 6, and also 7 if it is used) must be copied to a printer or some other device after the program terminates so they will not be lost. Sections 3.3.1 - 3.3.5 describe the information written to the different output files.

The program functions differently in some respects when only one line, rather than an entire band, is being considered. In particular, the thin-line bypass option is suppressed so that the full calculation is performed regardless of the optical depth along the path. With one line, no synthetic spectrum can be generated. However, the detailed radiance profile is printed out (along with the path optical depth) as a function of frequency as the numerical integration proceeds outwards, panel by panel, from the resonant frequency. Note that because of both the Gaussian integration and the panel-width adjustment for the wings (see Section 2.3.4.1), these points are not equally-spaced in frequency. There are other ways in which the printed output on units 4 and 5 differs as well.

3.3.1 UNIT 4: PRINCIPAL PROGRAM OUTPUT

The principal program output is written to unit 4. Examples appear in Appendixes A.4 and B.4.

NLTE first repeats the program input found in files TAPE1, TAPE2, and TAPE3, and also writes some subsidiary information. In the case of the atmospheric profile, the first seven variables in Table 3 are all printed as a function of altitude for the altitude range used in the calculations, even though one or two of them will have been calculated rather than read directly. It also prints the atmospheric pressure used to evaluate the Voigt lineshape (taken from a program database derived from the U.S. Standard Atmosphere, the vibrational temperature TVQ used to calculate the vibrational partition function, and the partition function itself.

When an entire band is considered, the integrated radiance is printed for each line and each viewing path. Two quantities are given: the result of the numerical integration over the radiance profile, under the heading "thick"; and the result which would be obtained if there were no absorption along the path ("thin"). Note that, for very thin lines, the latter is taken as the proper result and the thick calculation is bypassed. The principal results, the sum of the integrated radiance for all the lines, is then printed as "total band radiance." If a synthetic spectrum is generated, that is the last information written to unit 4.

Note that if there are more than five viewing paths, the program loops through them in groups of five, putting out the results sequentially. The synthetic spectrum for all paths still comes at the end.

As noted above, the program output for single-line runs is more detailed. The radiance and path optical depth are printed as a function of frequency, and the results of the integration over successive panels (designated P1, P2, etc.) are also written. The contribution from the tail of the radiance profile-the region from the last integration panel to infinity-talso appears. Differences in the output between single-line runs and band runs can be seen by comparing Appendixes A.4 and B.4.

3.3.2 UNIT 5: SUBSIDIARY PROGRAM OUTPUT

The output on unit 5 is quite detailed information—some of it physical and some of it just program parameters and indices—which can be used in various ways. Examples appear in Appendixes A.5 and B.5.

For a full band, the cumulative program execution time is given for each line. In addition, for each path, the cumulative band radiance and the path optical depth at the center of each line are printed. The latter is useful for estimating the effects of self-absorption along the paths. In addition, the indices LB, LL, and KM are printed. They are, respectively, the number of the first expanded integration

panel, the number of the last panel used, and the index of the highest-altitude layer used. LB is the same for all paths for a given line; the others may be different. LB and LL are zero for thin lines.

For single-line runs, two sets of altitude-dependent quantities are printed. Among them (in the first set) are the volume emission rate, the adjusted line strength KT, the Doppler width, the Lorentz-to-Doppler linewidth ratio RAT [y in Eq. (43)], and the Voigt function at the line center, \mathbf{f}_{ν_0} . In the second set are, for each path, the physical distance (in km) through each layer, the optical depth at the line center within each layer, and the contribution to the total observed radiance at the line center from each layer. The last two of these are useful for extimating the range of altitudes "observed" from the end of the path--that is, the depths from which radiation escapes along the viewing path, and the altitudes at which emission from deeper layers is effectively trapped. For limb-look, however, only the near half of the viewing path is evaluated for this purpose.

3.3.3 UNIT 6: DIAGNOSTIC INFORMATION

The information written to unit 6 is for diagnostic purposes only. Examples appear in Appendixes A.6 and B.6.

If peculiar program input is encountered, potential problems may be noted on unit 6. In normal operation, the headers on each of the input files are echoed, as is the first data card-image. Dummy format fields are juxtaposed for help in locating the faulty input. In the case of unit 2, the program's interpretation of the quantities on the lowest-altitude data card is given, in order to eliminate confusion about the input options and to identify the logical path taken by the atmospheric profile setup routine, ATMPR.

NLTE may also write other special messages, usually to make note of a change in some program parameter or procedure that might be needed to avoid an execution-time error. For example, if the synthetic spectrum array is in danger of being overfilled, NITE issues a warning and only calculates points falling within the allotted space. (In this particular case, the user can rerun the job with a larger value of DEL if important information is lost.)

3.3.4 UNIT 7: SYNTHETIC SPECTRUM

Unit 7, file SPECF, is read and written only when a synthetic spectrum is generated. The information on it is also written to unit 4; its purpose on output is to provide a file that can be saved and used as input to another program. "Another" program might be NLTE operating on an overlapping band (as discussed in Section 3.1), or it might be a program to read and plot the results of the final calculation.

The format of SPECF is such that NLTE can read it automatically. It starts

with a header card-image identifying the type of information on the file (band radiance). This is followed by header card-images identifying the molecule, isotope, band, and branch, with one card for each band contributing to the spectral radiance on the file. Each of these header cards also contains the date and time of the NLTE run that calculated that band's contribution.

The first data card-image gives the synthetic-spectrum and viewing path parameters used to generate the spectra contained on the file. It is there for NLTE to check parameters for consistency, but can be ignored by plot programs.

The second card-image gives the number of bands contributing to the spectra on the file, and the total integrated radiance due to all these bands.

The spectral radiance curves start at the third data card-image. For each wavelength or wavenumber (depending on the units used), there is one card-image giving this quantity followed by up to 12 radiance values, 1 for each viewing path. The format is (F10.3, 1X, 12E10.3).

An example of unit 7 output appears in Appendix A. 7.

3.3.5 UNIT 9: OUTPUT FOR INTERACTIVE USAGE

NLTE is a batch-oriented code in the sense that it requires input files to be prepared ahead of time. Since these files can be local, however, one often runs interactively. In such cases, it is useful to have output sent directly to the user, but the quantity of information written to unit 4 precludes the association of TAPE4 with OUTPUT, or at least makes the outcome less than satisfactory.

To surmount this difficulty, NLTE optionally defines an output file, unit 9, which is associated with the terminal (OUTPUT, on the CYBER). The information written to this file is a very limited subset of that written to unit 4. It includes enough information to identify successive stages of execution--specifically, reading the different input files--and also gives the principal output, the integrated radiance.

The procedure for making this feature optional relies upon a conditional-compile facility-using C\$ directives--which is available on the CYBER under NOS 2.3. It is invoked by using the DS parameter on the FTN5 control card. Under NOS, omission of this parameter results in no output to unit 9. Other compilers, however, will regard the C\$ directives as FORTRAN comments, with the result that unit 9 will be identified and used.

3.4 Transportability

In addition to extensive tests on the CYBER 750 on which the code was developed, NLTE test runs have been completed on a CRAY 1-A supercomputer and on a VAX 11/750 with a floating-point accelerator using VMS.

One set of modifications which is necessary in order for NLTE to run on other

systems involves replacing the calls to the CYBER system functions DATE, TIME, and SECOND. DATE and TIME are called in subroutine LINES, and the results are carried into SPECTRM. SECOND, which gives the elapsed processor time, appears in three places in the main program.

The limited dynamic range of FORTRAN variables which is imposed by some 32-bit machines can cause an overflow problem while evaluating the series representation of the Voigt function in region 1 of ZVGTC. (See Section 2.3.5.) The largest number which can appear there is approximately 10⁶⁶; on the VAX, the default range is only about 10^{±38}. This problem can be avoided by using VWERF instead of ZVGTC (set NDP = -1; see Section 3.2.1.3). Alternatively, with a VAX, one can use the /G_FLOATING option in ZVGTC to extend the dynamic range for the variables (AN, FNR, FNI, FPR, FPI) which require it, resulting in slower arithmetic for Region 1. If the /G_FLOATING format is implemented in software rather than hardware, the slowdown is considerable, and it is best to use VWERF or find some other alternative.

If underflow messages appear in the output, setting the symbolic constant EXPL equal to the largest argument the EXP function can handle without <u>overflowing</u> may eliminate them. For the VAX, we use EXPL =88.

The OPEN statements for units 1-6 (in subroutine LINES) do not contain the FILE= parameter. One uses job control language to associate input files with the logical units (e.g., GET on the CYBER under NOS 2.3, ASSIGN on the VAX and Cray). For unit 9, if it is used, the FILE= parameter must be set to terminal output (OUTPUT on the CYBER, SYS\$OUTPUT on the VAX).

The conditional-compile facility which activates unit 9 can be implemented on a VAX using the /D_LINES qualifier on the FORTRAN command, provided that the proper lines of code are prefixed with a D in column 1. These lines are the ones appearing between the lines prefixed with C\$ in NLTE, LINES, SPECTRM, and HEADER.

In our tests, NLTE ran approximately four times as fast on the Cray as on the CYBER, and seven times slower on the VAX than on the CYBER. In the latter comparison, VWERF rather than ZVGTC was used for the Voigt function. Fast-execute optimizations were utilized in all tests.

4. RESULTS

NLTE has been applied to many problems involving infrared transmission in the upper atmosphere, and has been used to simulate the SPIRE experiment 13 and other experiments. In this section, we illustrate the usefulness of the code by citing results from our model of solar-pumped emission from the CO $_2$ ν_1 + ν_3 combination bands near 2.7 μ m. 14

The most important physical mechanisms involved in this model are

- (1) solar pumping of the 101 and 201 levels from ground at 2.7 and 2.0 μ m, and of the 111 levels from the low-lying 010 level at 2.7 μ m;
- (2) collisional reorientation reactions which redistribute the populations among the directly-excited high-lying Fermi resonance split levels (e.g., 20011, 20012, 20013) and also to adjacent levels with different symmetry which are themselves not strongly pumped (12211, 12212);
- (3) V-V collisions with nitrogen molecules, the net effect of which is usually to quench the radiating levels; and
 - (4) spontaneous emission.

Details, including assumed reaction rates and an energy level diagram, can be found in Sharma and Wintersteiner. 14

We first used a solar-flux absorption code, SABS, which is similar in design to NLTE, to calculate the excitation rates at altitudes between 40 and 160 km due to absorption in all important infrared bands of CO_2 . We then assumed steady state conditions and equated the total radiative and collisional excitation rates with the total radiative and collisional de-excitation rates to get the number densities of all the high-lying states that emit at $2.7 \mu m$. Finally, we used NLTE to predict the observed radiance on limb paths between 50 and 100 km. Using an independent estimate of radiance due to water vapor, ¹⁴ we compared these results to the SPIRE database. Because the rate constants for the collisional reorientation reactions are poorly known, we also recalculated the radiance using adjusted values for these constants in order to identify the errors they might cause and set limits on their possible values.

Figure 5 gives, as a function of tangent height, the total CO_2 radiance in the 2.6 to 2.9 μ m region (solid squares) and the breakdown according to sets of contributing bands. The most important sets are the one with the resonant 10012-00001

Stair, A.T., Jr., Sharma, R.D., Nadile, R.M., Baker, D.J., and Grieder, W.F. (1985) Observations of limb radiance with cryogenic Spectral Infrared Rocket Experiment (SPIRE), J. Geophys. Res. 90:9763.

^{14.} Sharma, R.D., and Wintersteiner, P.P. (1985) CO2 component of daytime Earth limb emission at 2.7 micrometers, J. Geophys. Res. 90:9789.

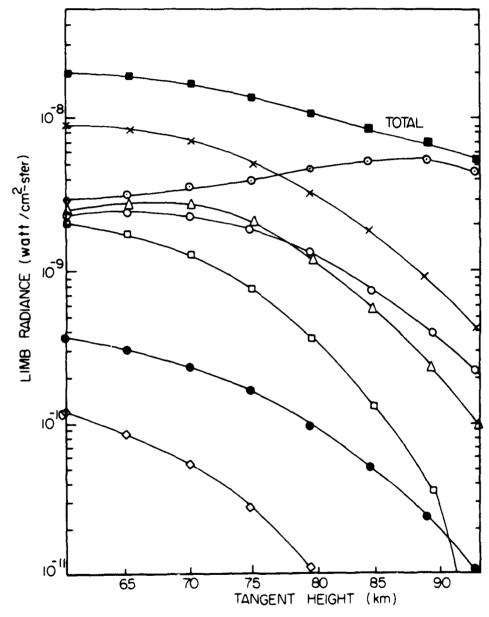


Figure 5. Predicted CO₂ Band Radiance in the 2.6 to 2.9 µm Range as a Function of Tangent Height. Circled dots represent the major-isotope resonant bands; crosses, the bands originating in the 201 levels; triangles, the bands originating in the 111 levels; open circles, minor-isotope resonant bands; open squares, bands originating in the 121 levels; solid circles, bands originating in the 301 levels; and diamonds, bands originating in the 221 levels

and 10011-00001 transitions (\odot) and the one with the transitions originating in the 20011, 20012, and 20013 levels (x). Lines in the resonant bands are very strongly self-absorbed on the lower viewing paths, in contrast to lines of the 2.7 μ m hot bands originating in the 201 levels, most of which are thin. For this reason, the latter group of bands provides the greatest contribution to the total radiance for viewing paths extending below 75 km. Above this altitude, the self-absorption is less and the resonant bands dominate. Groups of more weakly contributing bands in Figure 5 are discussed in Sharma and Wintersteiner. 14

Figures 6 and 7 give the spectral radiance as a function of wavelength. A triangular scanning function with a full width a ι half maximum of 0.038 μ m was used to produce these curves.

In Figure 6, the total radiance is plotted for different tangent paths. These curves are the summed output produced automatically on unit 7 by consecutive NLTE runs for all the contributing bands.

Figure 7 gives, for a tangent path of 75 km, the breakdown of the spectral radiance according to the groups of bands whose integrated contributions are shown in Figure 5. These curves are also summed output from unit 7, but selected differently.

Figure 8 gives the total spectral radiance for the 75 km tangent path, calculated using different assumptions about the collisional reorientation reaction rates. The basic model is the same curve as in Figure 7. "MOD1" decouples some of the high-lying levels, and "MOD2" is the extreme case of decoupling all these levels. (Other modifications involved coupling that was somewhat weaker, or somewhat stronger, than that of the basic model.) One can see that the NLTE radiance predictions are quite distinct—distinct enough, in fact, that a comparison with the SPIRE experiment allows us to rule out the more extreme modifications completely and to put lower limits on the principal rate constants.

The comparison with the experiment is given in Figures 9 and 10. Although the spectral fit is not perfect, the discrepancies together with a detailed examination of the physical mechanisms involved indicate the direction in which the coupling may be adjusted. In general, it is true that most of the conclusions derived from this and other similar modeling efforts rely upon comparing the total predicted radiance with experimental values. In this way--by use of an accurate and efficient radiance code, like NLTE--one can obtain a great deal of information about the physical processes involved in exchange of energy among excited vibrational levels of one or more molecular types.

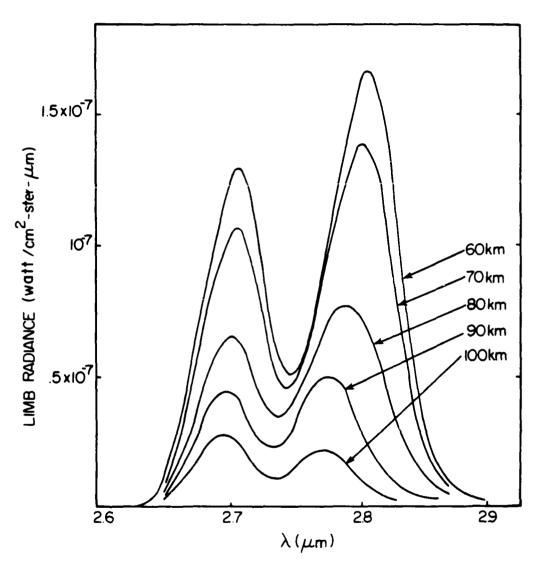


Figure 6. Spectral Distribution of ${\rm CO_2}$ Limb Radiance for Tangent Heights Between 60 and 100 km

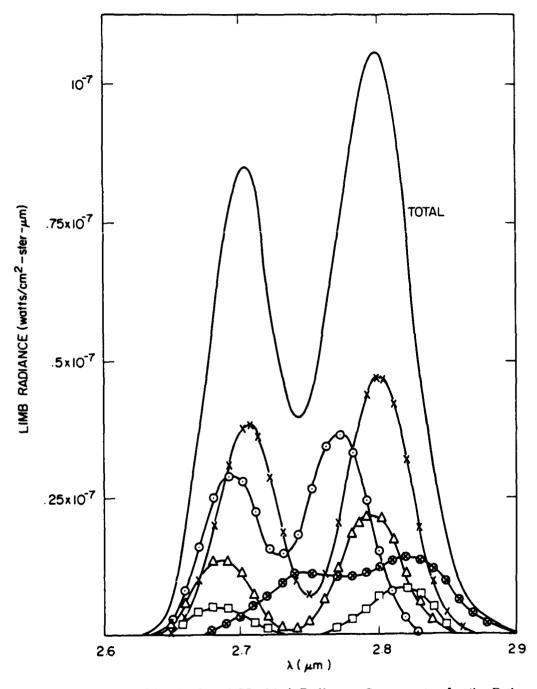


Figure 7. Spectral Distribution of CO2 Limb Radiance, Components, for the Path With a Tangent Height of $75\,\mathrm{km}$

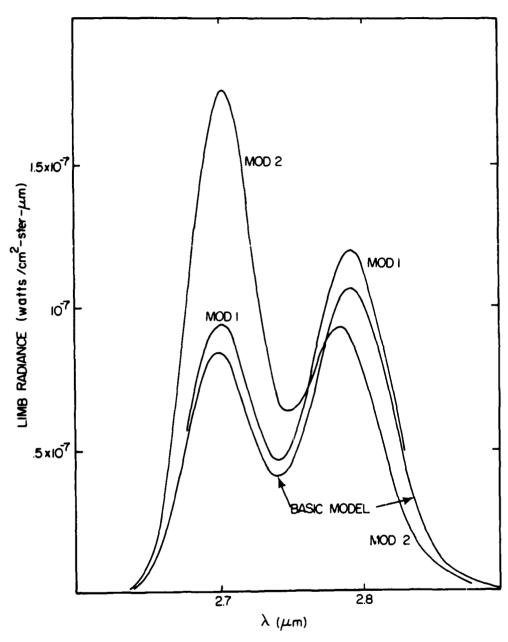


Figure 8. Spectral Distribution of Limb Radiance, From the Basic Model and From Two Modifications, for a Path With a Tangent Height of 75 km

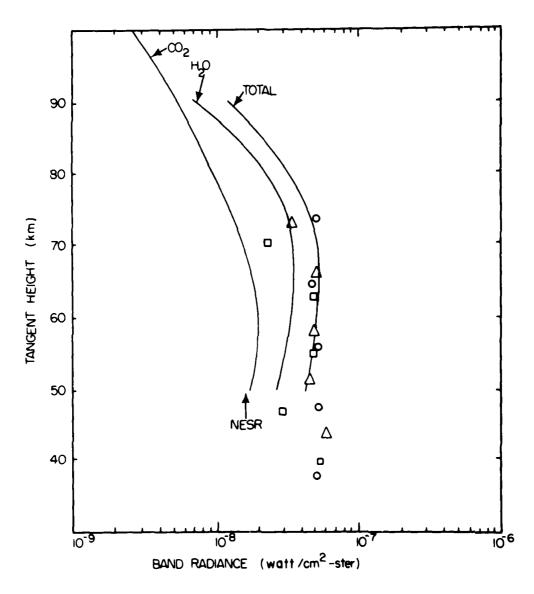


Figure 9. Comparison of Predicted and Experimental Band Radiance, 2.5 to 2.9 μ m, From SPIRE; and the Results of the CO₂ Model, ¹⁴ the H₂O Model, and Their Total. The detector noise limit is indicated by the arrow

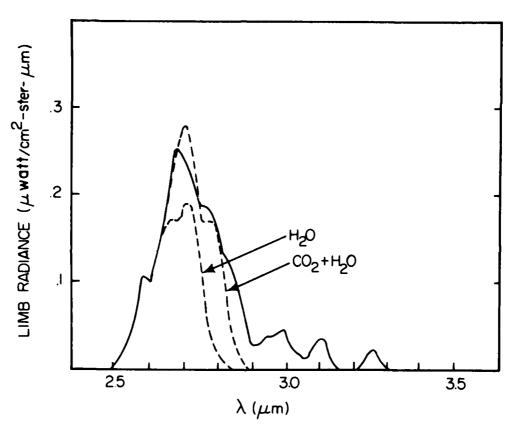


Figure 10. Comparison of Predicted and Experimental Spectral Radiance From the SPIRE Experiment (Solid Line) With Predictions of Contributions From CO2 and $\rm H_2O_{\bullet}$ for a Tangent Path of $73\,\rm km$

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Appendix A

Sample Run 1: Band Radiance

Appendix A contains Sample Run 1, in which the limb radiance due to the low lying 02201-01101 hot band of ${\rm CO}_2$ is calculated for five viewing paths with tangent heights between 70 and 90 km. The "top" of the atmosphere was assumed to be at 150 km, and a maximum of 80 layers was used. The program required a fractional error of 1 percent or less for each line, used two integration points per panel, and ran in 17 sec on the CYBER 750 at AFGL. (Using four integration points per panel, the same job takes 28 sec.) Synthetic spectra were generated for each of the viewing paths and were added to spectra previously calculated and stored on a permanent file, due to the ν_2 fundamental (01101-00001) from the 626, 636, and 628 isotopes.

The results for the total band radiance for the five paths differ from those of a similar run specifying much greater accuracy and eight integration points per panel by 0.14 percent, 0.09 percent, 0.41 percent, 0.87 percent, and 1.01 percent. This indicates that (for this example, at least) the mathematical approximations utilized in the code perform properly.

The physical approximation introduced by the homogeneous atmospheric layers is, of course, not addressed by this comparison. However, as discussed in Section 2.3.4.3, we expect the resultant errors to be on the order of, or less than, the values given above.

A1. Unit 1: Input for Sample Run 1

```
'CO2', 626, '02201', '01101'/
70, 90, 5
150, .01, 2/
.27, .05, 'UM'
```

A2. Unit 2: Input for Sample Run 1

The beginning of the file defining the atmospheric profile used for Sample Run 1 is given below. The file contained data for altitudes between 65 and 249 km, but was only read to 150 km. The first five altitudes were also ignored (because the lowest tangent height was 70 km) except that the input option was determined from the 65-km data. Option 7 was used because the fifth and sixth data fields both contain vibrational temperatures.

```
CA0402S
         ATMOS PROFILE 7/16/85
C
         ALT, TRTMP, RHO, TVL, TVU, TVQ---ALL TVS SAME AS ON A0201S
С
         VIB TEMPS FROM BULLITT'S NU2 MODELLING USING O QUENCHING
CCO2
          02201
                    01101 65-249 KM
   65
        233.294
                  .10397E+13
                              .22829E+03
                                            .22829E+03
                                                         .22829E+03
   66
        230.554
                  .90856E+12
                              .22482E+03
                                           .22482E+03
                                                        .22482E+03
        227.814
                  .79397E+12
   67
                               .22136E+03
                                            .22136E+03
                                                         .22136E+03
  68
        225.074
                  .69383E+12
                               .21783E+03
                                            .21783E+03
                                                         .21783E+03
                  .60632E+12
  69
        222.334
                              .21424E+03
                                            .21424E+03
                                                         .21424E+03
  70
        219.590
                  .52965E+12
                              .21176E+03
                                            .21176E+03
                                                         .21176E+03
        217.350
                  .45791E+12
  71
                               .20853E+03
                                            .20853E+03
                                                         .20853E+03
  72
        215.110
                  .39589E+12
                              .20522E+03
                                            .20522E+03
                                                         .20522E+03
  73
        212.870
                  .34227E+12
                              .20184E+03
                                            .20184E+03
                                                         .20184E+03
  74
        210.630
                 .29591E+12
                              .19839E+03
                                           .19839E+03
                                                         .19839E+03
        208.381
  75
                  .25561E+12
                              .19487E+03
                                            .19487E+03
                                                         .19487E+03
  76
        206.421
                  .21893E+12
                              .19146E+03
                                            .19146E+03
                                                         .19146E+03
  77
        204.461
                  .18752E+12
                              .18804E+03
                                            .18804E+03
                                                         .18804E+03
  78
        202.501
                  .16061E+12
                              .18460E+03
                                            .18460E+03
                                                         .18460E+03
        200.541
  79
                  .13756E+12
                              .18119E+03
                                            .18119E+03
                                                         .18119E+03
  80
        198.558
                  .11759E+12
                              .17780E+03
                                            .17780E+03
                                                         .17780E+03
  81
        196.618
                 .10004E+12
                              .17445E+03
                                            .17445E+03
                                                         .17445E+03
  82
        194.678
                 .85113E+11
                              .17122E+03
                                           .17122E+03
                                                         .17122E+03
  83
        192.738
                 .72413E+11
                              .16814E+03
                                            .16814E+03
                                                         .16814E+03
  84
        190.798
                 .61608E+11
                              .16525E+03
                                           .16525E+03
                                                         .16525E+03
  85
        188.886
                 .52136E+11
                              .16256E+03
                                            .16256E+03
                                                         .16256E+03
  86
        188.606
                 .43675E+11
                              .16082E+03
                                           .16082E+03
                                                        .16082E+03
        188.326
                 .36587E+11
                              .15933E+03
                                           .15933E+03
                                                        .15933E+03
```

A3. Unit 3: Input for Sample Run 1

The beginning of the file containing the transitions needed for Sample Run 1 is given below. That data corresponding to isotopes other than the one of interest are ignored.

```
CL020010 CO2 ALL 02201
590.07000 3.750E-27.0550
591.51830 6.585E-27.0550
592.96930 1.138E-26.0560
594.42310 1.936E-26.0560
594.74740 5.111E-27.0550
595.98850 8.892E-27.0550
597.23860 1.523E-26.0560
597.33930 5.342E-26.0560
597.33930 5.342E-26.0560
598.49760 2.567E-26.0570
598.80170 8.663E-26.0580
599.48690 4.198E-27.0500
                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        5/85 1
02201
02201
02201
02201
02201
                                                                                                                                                                                                                                                                                                                                                                                                                                        01101 08/
3054 161
2933 382
2815 695
2701 102
2989 619
2589 604
2870 575
2754 619
2481 203
2641 754
2375 902
2401 203
2641 754
2375 902
2405 001
2531 980
2273 702
3862 635
2425 300
2273 702
3862 635
2425 300
2531 715
2078 612
2221 227
3587 135
1985 725
2123 838
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A4. Unit 4: Output From Sample Run 1

The principal program output from Sample Run 1 is given on the following 15 pages.

```
PROGRAM NUTE FOR INFRARED RADIANCE
DATE + 85/09/04. TIME = 09.21.02.
TACEL
TUTTP12---SAMPLE RUN 1, TAPE1---CO2 NH2 15UM 626 HOT BAND
IA- -: INE DIRECTIVES:
MOL = MOLECULE CODE = CO2

ISO = ISOTOPE CODE = 626

IN1 = UPPER VIB LVL = 02201

EN1 = LOWER VIB LVL = 01101

BII = RO-VJB BRANCH = 10101
 NRL - ROT'L LINE .
 III---VIEWING PATH PARAMETERS:
TAN1 = LOWEST TANGENT HEIGHT (HM) = 70.00
TANF = HIGHEST TANGENT HEIGHT (HM) = 90.00
SPAL = EXAMINATION INTERVAL (HM) = 5.00
LOOK = 0: LOOKING GEOMETRY CHOSEN = LIMB
 IC --- PRUGRAM PARAMETERS:
HMAX = ASSUMED TOP OF ATMOSPHERE (RM) = 150
ACC = ACCURACY (INTEG D RADIANCE) = .01000
NPTS = NUMBER OF INTEG POINTS PER PANEL = 2
HIDP = 0; LINESHAPE OPTION SELECTED = VOIGT
VALUE = LOWER END, LINE SEARCH (CM-1) = 0
VALAK = UPPER END, LINE SEARCH (CM-1) = 70000
 10--- SYNTHETIC SPECTRUM PARAMETERS:
 FWHM = WIDTH OF TRIANGULAR SCANNING FN (UM ) = UEL = SPACING OF PTS IN SYNTH SPECTRM (UM ) =
 1E -- BAND PARAMETERS: (FOUND IN MOLPAR)
 VIBE = VIB ENERGY OF THE TRANSITION (CM-1) = 667.7500
VIDI. = VIB ENERGY OF THE LOWER STATE (CM-1) = 667.3790
VIDI = QUANTUM FOR THE PARTITION FN (CM-1) = 667.3790
GL = STATISTICAL WEIGHT, LOWER VIBRATIONAL STATE = 2
 QUANTITIES RETURNED FROM MOLEC:
 WGT = MOLECULAR WEIGHT = 44
A1 = ISOTOPIC ADUND = .98414
OLIGO (EXPLAINED IN MOLEC) = 1.0
IFAD (EXPLAINED IN MOLEC) = 1.0
IFAD (EXPLAINED IN MOLEC) = .25
 FIRMAL FOR THE SEARCH OF THE LINETAPE IS OF THE LINETAPE IS
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37010

AIMOS PROFILE 7/16/85 ALT. TRIMP.RHO,TVL,TVU,TVU,TVG-- ALL TVS SAME AS ON AO2015 VIÐ TEMPS FROM BULLITT'S MUZ MODELLING USING O QUENCMING AND SPIRE DATA 02201 - 01101 - 65-249 KM INPUT OFFICH # 7: NVP + 1, NPF - 1, VIBL > 0; (SEE COMMENTS IN ATMPRS 60.

LIVE LINWER AND UPPER-STATE POPULATIONS REFLECT AN ABUNDANCE OF .98414 W.R.T. TOTAL CO2

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2. 1893 E-11
7. 1891 E-11
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5.1508E*10 3.6100E*08 1.0777E*05 165.250 1 4.1575E*10 2.1826E*08 1.5283E*05 165.250 1 1 3796E*08 1.5583E*05 1589.330 1 37055E*10 1.3829E*08 1.1501E*05 159.330 1 37055E*10 1.3829E*08 1.1501E*05 158.330 1 37055E*10 1.3829E*08 1.1501E*05 158.330 1 37055E*10 1 3729E*08 1.1501E*05 158.330 1 3729E*10 1 3277E*07 1 3729E*05 158.300 1 3729E*10 1 3729E*07 1 3729E*05 158.300 1 3729E*07 1 3729E
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SHURDDITINE SPECTRM RECOGNIZES FILE WITH PREVIOUSLY-CALCULATED BAND RADIANCES; WILL ADD TO THIS DATA-BASE

33 17.400 ININ - TEMPERATURE USED FOR STOW = 188 SIU HOPP WIDIH = STOW (CM-1) = .49441E-03 Z FI GAUSS QUADRATURE USED FOR HY-INTEG THAK = 88, RANGE = 13.050 TO

276 LIMES

TIME FOR INITIALIZATION : 3 19 SEC.

GROUP # 1 WITH S VIEWING PATHS

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5 VIEWING PATHS AND 4 COZ BANDS 7.420E-07 80.00 75.00 KM 2427E-13 2427E-13 2426E-13 2426E-13 2426E-13 2426E-10 242 3 RADIANCE SPECTRUM FWIN FOR TRIANGULAR SUBBOUTINE SPECTRM: 70.00 (INTEG-TD) WL (UM) 

3

15.550 1.301E-00 6.029E-07 3.258E-07 1.000E-07 1.236E-07 15.550 0 3.242E-07 3.099E-07 1.256E-07 1.254E-07 1.256E-07 
# A5. Unit 5: Output From Sample Run 1

Subsidiary program output from Sample Run 1 begins on the next page.

FROGRAM NETE FOR INFRARFO RADIANCE DATE - RS/09/04, TIME 1 09-21-02.

145Ff.S.

CUMULATIVE INFEGRATED RADIANCE (WATT/CM2*STR) AND TOTAL OPTICAL DEPTH (AT LINE CENTER) FOR VARIOUS LINE-OF SIGHT PATHS

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90.00KM	186.1	3336-14	07E-1	.989E-14	- 36	36-1	7.6 - 1	3006-13	-	9E-1	536-1	45E-1	. 934E - 13	26-1		85E-1	086-1	57E-1	86E-1			100	79E-1	759E-12	3.6	105F-11	1000		M.J	2366-11	. 291E-11	175	485E-11	ROBE-11	300		01.3601.	Ξ,	28 - 1	27RF 10	3626-10	4546-10	5491-10
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85.00 KM	126-1	176-1		940E-14	7	83E-1	536-1		28E-1	-	21E-1		186-1	1	7	E-1	1	- ₩.		~ -		-	_	-	ш.	1135-11			2516-11	7956-11	4605-11	6126-11	7326-11	_			-	7	- 1	5196-10	475-1	2E - 0	E-0
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0P 0PTH L	169E - 06	505	35	- 0	980	313E-06		OE '	05	2	1416-05	4	-	519E-05	9	990		155			, .	978	960		- 0			•	~ .		9	4	<b>L</b>	v i		335	_	9	<u>س</u> ز	145E + 00	0E • 0	7E • 0	1571.00
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0.0 0.114	243E-0		o c	3806-0	ę,	830E-0	27E-		į.		0-14/6	<u>.</u>	6E -	2E -	2	9	7436-0		LABE-D		96		•		4086-0				2505.0	- 7		٠	45-0	1776	0	0	35 + 0	0	7126.0	0	Ė	ů	1356.0
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70.	. 1536	409	1746	348	. 3686	7855	. 830£	1605	1728	.3358	2005	1576	1476	1595	3076	3316	2705	7000	1385	. 1595	. 275E	3188	5386		1001	1945	. 225E	3576		744	920	Ē.		2776	373	454	. 805	729		14 3 E	3	201	2418
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EXFC 11MF				3 30																										•	3 96	4 02	0.0		4 73	4 23	V.		4.52	4.59	4.65	4.71	4./7

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\begin{array}{c} -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- + 0 \\ -- +
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 $\begin{array}{c} c_1 + c_2 + c_3 + c_4 + c_4 + c_5 + c_4 + c_5 + c_4 + c_5 + c_4 + c_5 +$  $\sigma$ 

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\begin{array}{c} \mathbf{74} + \mathbf{60} +
```

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DDCDDCDCDCDCDCDCDCDCDCDCDCDCDCDCDCDC
```

## A6. Unit 6: Output From Sample Run 1

Diagnostic program output from Sample Run 1 is given on the next page. No extraordinary conditions were encountered; therefore, this output is confined to listing headers and card-images from the four input files.

UNIT 1;	(HEADER)
CICJTP12SAMPLE RUN 1, TAPE1COZ MUZ 15UM 626 HOT BAND	(FORMAT)
1111111112272222223333333344444444444444	(DATA)
UNIT 2: CAGGOSS ATMOS PROFILE 7/16/65 C ALT.TRIMP.RHO.TVL.TVU,TVQALL TVS SAWE AS ON AD201S C VIB TEMPS FROM BULLITT'S NUZ MODELLING USING O QUENCHING AND SPIRE DATA CC2 GZZOT OFIOT OFIOT OFIOT S2249 HT. AAAAABBBBBBBBCCCCCCCCCCCCCCCCCCCCCCCCC	(HEADER) (HEADER) (HEADER) (HEADER) (FORMAT) (DATA)
UNIT 3:	(HEADER)
CLO20010 COZ ALL 02201 0:101 08/15/85 ;5UM NUZ HOT BAND	(FORMAT)
1:111111112222222222222333333334444444444	(DATA)
UNIT 7:  CXXXXXXX BAND RADIANCENLTE OUTPUT  CC02 626 01101 00001 A 65/09/04. 08.53.03.  CC02 626 01101 00001 A 85/09/04. 08.55.01.  CC02 636 01101 00001 A 85/09/04. 08.55.53.  CC02 638 01101 00001 A 85/09/04. 08.55.53.  IIIIIII111111122222222233333334444444444	(HEADER) (HEADER) (HEADER) (HEADER) (HEADER) (FORMAT)

TAPES

PROGRAM NLIE FOR INFRARED RADIANCE Paie = 85/09/04, TIME * 09.21.02. PRINI THE HEADERS AND FIRST DATA CARO-IMAGES FOUND ON INDUT UNITS

### A7. Unit 7: Output From Sample Run 1

The unit 7 output from Sample Run 1 is given below. Note that the information, although not given in the same format, is the same as that given at the end of unit 4.

```
CXXXXXX BAND RADIANCE
                              --- NLTE OUTPUT
CCO2 626
CCO2 636
                     00001 A --- 85/09/04. 08.53.33.
            01101
                      00001 A --- 85/09/04. 08.55.01.
            01101
                     00001 A --- 85/09/04. 08.55.53.
01101 A --- 85/09/04. 09.21.02.
CCO2 628
            01101
CCO2 626
270
            02201
              .050 UM LIMB LOOM: HTS (KM) = 70.00 75.00 B
3.171E-06 1.514E-06 7.420E-07 4.029E-07 2.798E-07
4.242E-15 4.356E-15 4.531E-15 4.733E-15 4.965E-15
                                                            75.00 80.00 85.00 90.00
             .050 UM
     13.050
              3.992E-14 4.070E-14 4.231E-14 4.421E-14 4.639E-14
     13.100
     13.150
              1.444E-13
                         1.446E-13 1.502E-13 1.570E-13 1.647E-13
                         3,652E-13 3.778E-13 3.947E-13 4.145E-13
              3.786E-13
                         7.791E-13 7.996E-13 8.352E-13 8.775E-13
     13,250
              B.678E-13
                         1.593E-12
                                    1.600E-12 1.668E-12
              2.075E-12
     13 , 300
                                                           1.754E-12
                                    2.955E-12
              5.234E-12
                         3.096E-12
                                               3.065E-12
                                                           3.222E-12
     13 350
              1.419E-11
                                    5.229E-12
                                               5.359E-12 5.630E-12
     13.400
                         6.058E-12
     13,450
              4.517E-11
                         1.335E-11
                                    9.37BE-12
                                               9.290E-12 9.730E-12
     13 500
              1.382E-10
                           . 168E-11
                                    1.687E-11 1.565E-11 1.626E-11
     13.550
              4.422E-10 8.802E-11 3.329E-11 2.702E-11 2.750E-11
     13,600
                         2.521E-10
                                    7,173E-11 4,734E-11 4,6:6E-11
              1.325E-09
                         7 097E-10
                                    1.683E-10 8.685E-11 7.852E-11
     13.650
              3.648E-09
                         1.979E-09 4.324E-10 1.740E-10
     13,700
              9.222E-09
                                                           1.3958-10
              1.961E-08 4.807E-09 1.064E-09 3.599E-10 2.521E-10
     13 750
                         1 068E-08 2.631E-09
                                               8.189E-10 4.962E-10
              3.698E-08
     13 800
     13 850
              6.097E-08
                         1.9898-08 5.5628-09
                                               1,7468-09 9.6268-10
     13,900
              9.2888-08
                         3.353E-08
                                    1.075E-08 3.694E-09
     13,950
              1 312E-07
                         5.072E-08
                                    1.802E-08
                                               6.824E-09
                                                           3.714E-09
     : 4.000
                750E-07 7.137E-08 2.769E-08 1.163E-08 6.703E-09
     14.050
              2.241E-07 9.433E-08 3.911E-08 1.792E-08 1.095E-08
                         1.190E-07 5.179E J8 2.579E-08 1.68DE-08
1.464E-07 6.517E-08 3.471E-08 2.392E-08
              2.786E-07
     14,100
              3.402E-07
     14,150
              4.102E-07
                         1.770E-07
                                    7.930E-08 4.430E-08 3.224E-08
     14.200
              4.890E-07
                         2.127E-07 9.491E-08 5.435E-08 4.117E-08
     14,250
              5.796E-07
                         2.543E-07
                                    1.128E-07 6.490E-08 5.052E-08
     14,300
              6.799E-07
                         3.015E-07
                                    1.336E-07 7.616E-08 6.002E-08
     14.350
                                    1.578E-07 8.831E-08 6.952E-08
     14.400
              7.909E-07 3.542E-07
     14.450
              9.095E-07 4.109E-07 1.853E-07 1.017E-07 7.912E-08
              1.031E-06 4.686E-07 2.149E-07 1.160E-07 B.843E-08
```

```
1.150E-06 5.266E-07 2.459E-07 1.313E-07 9.778E-08 1.257E-06 5.803E-07 2.759E-07 1.463E-07 1.063E-07
14 550
14.500
        1.357E-06 6.321E-07 3.052E-07
                                         1.609E-07
14.650
                                                    1.143E-D7
        1.514E-06
                   7.135E-07 3.485E-07
                                         1.837E-07
                                                    1.280E-07
14.700
14.750
        2.050E-06 9.619E-07 4.769E-07
                                         2.585E-07
14,800
        2.596E-06
                   1.209E-06 6.039E-07 3.345E-07 2.399E-07
                   1.496E-06 7.471E-07 4.161E-07
14 850
        3 217F-06
                                                   2.990F-07
14.900
        3.862F-06
                   1.798E-06 8.972E-07 5.010E-07
                                                   3.601E-07
14.950
        4.427E-06
                   2.059E-06
                              1.028E-06 5.771E-07 4.158E-07
        4.384E-D6 2.04GE-06
                              1.020E-06 5.709E-07 4.084E-07
15,000
15.050
        3.979E-06
                   1.883E-06 9.354E-07 5.146E-07 3.606E-07
15.100
        3.4918-06
                   1.682E-03 8.366E-07 4.534E-07 3.110E-07
15.150
        2.859E-06 1.393E-06
                              1.941E-07 3.730E-07 2.532E-07
        2.303E-06 1.151E-06 5.783E-07 3.078E-07
                                                   2 D49F-07
15,200
        1.881E-06 9.742E-07 4.935E-07 2.593E-07
15, 250
                                                    1.686E-07
15,300
        1.828E-06 9.529E-07 4.867E-07 2.597E-07
                                                    1.714E-07
15.350
        1.762E-06 9.216E-07 4.723E-07
                                        2.558E-07
                                                    1 715E-07
        1.767E-06 9.326E-07 4.779E-07 2.610E-07
15 400
                                                    1.751E-07
15,450
        1.642E-06 8.632E-07 4.373E-07
                                        2.398E-07
                                                   1.6198-07
15.500
        1.474E-06 7.655E-07 3.815E-07 2.098E-07 1.424E-07
15.550
        1.301E-06 6.629E-07 3.258E-07
                                         1.806E-07 1.236E-07
15.600
        1.113E-06 5.539E-07 2.696E-07 1.514E-07 1.041E-07
15.650
        9.242E-07 4.464E-07 2.158E-07 1.224E-07 8.440E-08
15.700
        7.829E-07 3.699E-07 1.791E-07 1.015E-07 6.884E-08
        6.816E-07 3.236E-07 1.601E-07 9.031E-08 5.947E-08
15 750
        5.902E-07 2.842E-07 1.429E-07 7.874E-08 4.978E-08
15.800
```

5.096E-07 2.506E-07 1.263E-07 6.678E-08 4.012E-08 4.399E-07 2.205E-07 1.090E-07 5.448E-08 3.085E-08 3.825E-07 1.933E-07 9.225E-08 4.310E-08 2.294E-08 15,850 15.900 15.950 16,000 3.323E-07 1,660E-07 7,511E-08 3.258E-08 1.631E-08 2.856E-07 1.384E-07 5.868E-08 2.414E-07 1.117E-07 4.408E-08 16.050 2.35BE-08 1.113E-08 16.100 1.643E-08 7.376E-09 1.981E-07 8.640E-08 3.154E-08 1.096E-08 4.738E-09 1.566E-07 6.382E-08 2.161E-08 7.082E-09 2.984E-09 16,150 16.200 16.250 1.192E-07 4.516E-08 1,423E-08 4,427E-09 1.833F-09 16.300 8.642E-08 3.039E-08 8.926E-09 2.647E-09 1.0868-09 16,350 6.017E-08 1.974E-08 5.455E-09 1.561E-09 6.422E-10 1.223E-08 3.180E-09 8.840E-10 3.684E-10 7.116E-09 1.749E-09 4.764E-10 2.038E-10 16.400 4.003E-08 16.450 2.513E-08 1.511E-08 3.993E-09 9.373E-10 2.530E-10 1.125E-10 16 500 16 550 8.601E-09 2.168E-09 4.916E-10 1.332E-10 6.221E-11 16.600 4.706E-09 1.115E-09 2.458E-10 6.751E-11 3.373E-11 2.389E-09 5.402E-10 1.163E-10 3.303E-11 1.810E-11 16.650 1,209E-09 2.637E-10 5.587E-11 1.685E-11 1.018E-11 16.700 16.750 5.932E-10 1.250E-10 2.640E-11 8.662E-12 5.800E-12 2.764E-10 5.62BE-11 1.207E-11 4.447E-12 3.304E-12 16.800 1.211E-10 2.397E-11 5.357E-12 2.308E-12 1.900E-12 5.418E-11 1.052E-11 2.499E-12 1.249E-12 1.105E-12 16.850 16.900 1-.950 2.377E-11 4.563E-12 1.180E-12 6.810E-13 6.359E-13 9.953E-12 1.908E-12 5.66E-13 3.706E-13 3.609E-13 3.937E-12 7.681E-13 2.634E-13 2.003E-13 2.011E-13 17.000 17.050 1.557E-12 3.171E-13 1.304E-13 1.098E-13 1.125E-13 6.327E-13 1.416E-13 7.173E-14 6.547E-14 6.792E-14 17 100 17 150 17,200 2.462E-13 6.311E-14 3.871E-14 3.726E-14 3.893E-14 8.992E-14 2.731E-14 1.960E-14 1.952E-14 2.047E-14 17.250 8.843E-15 9.293E-15 8.843E-15 9.293E-15 8.673E-15 3.710E-15 3.215E-15 3.299E-15 3.469E-15 1.528E-15 7.298E-16 6.577E-16 6.784E-15 7.137E-16 17.300 17.350 17,430

### A8. Command File for Sample Run 1

The following CYBER commands access permanent files (containing the NLTE binary and the input data), run the program, and copy the results to a line printer. The commands following EXIT allow for abnormal termination.

```
JOB. . .
USER...
CHARGE. . .
COMMENT.
COMMENT.
            NLTE SAMPLE RUN 1
                                     AUGUST 1985
            CO2 626 02201-01101 HOT BAND 15UM
COMMENT.
COMMENT.
            ADD SYNTH SPECTRA FROM NU2 FUND'LS
COMMENT.
GET, BIN=NLTEBIN.
GET, TAPE1=TC3TP12, TAPE2=A0402S, TAPE3=L020010, SPECF=SAMP2DP.
BIN.
COPYCF (TAPE4, OUTPUT)
COPYCF (TAPES, DUTPUT)
COPYCF (TAPE6, OUTPUT)
COPYSBF (SPECF, OUTPUT)
EXIT.
REWIND (TAPE4, TAPE5, TAPE6, SPECF)
COPYCF (TAPE4, DUTPUT)
COPYCF (TAPES, OUTPUT)
COPYCF (TAPE6, OUTPUT)
COPYSBF (SPECF, OUTPUT)
```

## Appendix B

Sample Run 2: Single Line

Appendix B contains Sample Run 2, in which the limb radiance due to a single ro-vibrational transition in one of the 101 combination bands of  $CO_2$  near 2.7 $\mu$ m is evaluated. Four viewing paths with tangent heights between 70 and 100 km are considered. The line chosen is one of the thickest lines in the band. The job ran in 2.6 seconds on the CYBER 750. Devault values were used for all program parameters. The errors for the radiance (determined as in Appendix A) are 0.10%. .057%, 0.06%, and 0.41% for the four viewing paths.

### B1. Unit 1: Input for Sample Run 2

```
'CO2', 626, '10012', '00001', 'R', 14
70, 100, 10
/
```

PRECEDING PAGE BLANK-NOT FILMED

#### B2. Unit 2: Input for Sample Run 2

The beginning of the file defining the atmospheric profile used for Sample Run 2 is given below. The file contained data from 40 to 160 km; only that at 70 km or above was used, except that the input option was determined from the 40-km data. Input option 3 was used in this case because the information in fields 3-6 consists of number densities.

```
CA1701
         ATMOS PROFILE 06/10/85
         ALT, TRTMP, NL, NU, NO, N1---DATA FROM VSIM, IRR---FORMERLY AT101G1
CCO2 626
           10012
                    00001
                           40-160 KM
                                            .25034E+14
        251.060
                  .25034E+14
                               .25415E+05
   40
                                                          .10925E+13
   41
        253.435
                  .21636E+14
                               .26519E+05
                                            .21636E+14
                                                          .97831E+12
                  .18700E+14
                               .27670E+05
        255.810
                                                          .87605E+12
   42
                                            .18700E+14
        258.185
                  .16213E+14
                               .28737E+05
                                            .16213E+14
                                                          .78596E+12
   43
                               .29846E+05
                  .14056E+14
   44
        260.560
                                            .14056E+14
                                                          .70513E+12
        262.150
                  .12230E+14
                               .29159E+05
                                            .12230E+14
   45
                                                          .62725E+12
        263.740
                               .28487E+05
                  .10641E+14
   46
                                            .10641E+14
                                                          .55797E+12
   47
        265.225
                  .93127E+13
                               .27679E+05
                                            .93127E+13
                                                          .49831E+12
   48
        266.710
                  .81506E+13
                               .26893E+05
                                            .81506E+13
                                                          .44503E+12
   49
        266.930
                  .71968E+13
                               .24042E+05
                                            .71968E+13
                                                          .39409E+12
   50
        267.150
                  .63547E+13
                               .21494E+05
                                            .63547E+13
                                                          .34899E+12
                  .56342E+13
   51
        265.555
                               .16974E+05
                                            .56342E+13
                                                         .30273E+12
        263.960
                  .49955E+13
   52
                               .13404E+05
                                            .49955E+13
                                                         .26260E+12
   53
        261.210
                  .44582E+13
                               .98753E+04
                                            .44582E+13
                                                         .22544E+12
   54
        258.460
                  .39787E+13
                               .72756E+04
                                            .39787E+13
                                                          .19354E+12
   55
        255.705
                  .35421E+13
                               .54637E+04
                                            .35421E+13
                                                         .16544E+12
                               .41031E+04
  56
        252.950
                  .31535E+13
                                            .31535E+13
                                                         .14142E+12
  57
        250.200
                  .28003E+13
                               .32335E+04
                                            .28003E+13
                                                         .12038E+12
  58
        247.450
                  .24867E+13
                               .25482E+04
                                            .24867E+13
                                                         .10247E+12
  59
        244.700
                  .22024E+13
                               .21592E+04
                                            .22024E+13
                                                         .86823E+11
  60
        241.950
                  .19506E+13
                               .18295E+04
                                            .19506E+13
                                                         .73564E+11
  61
        239.200
                  .17228E+13
                               .16620E+04
                                            .17228E+13
                                                         .62027E+11
  62
        236.450
                  .15215E+13
                               .15098E+04
                                            .15215E+13
                                                         .52299E+11
  63
        233.695
                 .13399E+13
                               .14565E+04
                                            .13399E+13
                                                         .43868E+11
                               .14051E+04
  64
        230.940
                 .11800E+13
                                            .11800E+13
                                                         .36796E+11
  65
        228.190
                 .10360E+13
                               .14114E+04
                                            .10350E+13
                                                         .30704E+11
  66
        225.440
                  .90964E+12
                               .14178E+04
                                            .90964E+12
                                                         .25620E+11
                               .14649E+04
  67
        222.690
                 .79611E+12
                                            .79611E+12
                                                         .21262E+11
  68
        219.940
                 .69675E+12
                              .15135E+04
                                            .69675E+12
                                                         .17645E+11
  69
        218.050
                 .60752E+12
                               .16079E+04
                                            .60752E+12
                                                         .14807E+11
  70
        216.160
                 .52972E+12
                              .17081E+04
                                            .52972E+12
                                                         .12425E+11
```

### B3. Unit 3: Input for Sample Run 2

The beginning of the file containing the 10012-00001 transitions needed for Sample Run 2 is given below. Ro-vibrational lines corresponding to bands or isotopes which are not needed are ignored. In fact, since this is a single-line run, the file could consist of just the one card-image corresponding to the transition under consideration.

CL101000 CO2 ALL 10012	00001 06/2	21/85 2	.7UM REGULAR	101 COMBINATION BANDS	
C 10011	00001				
3434 . 7011 3.607E-27.0590	1482.576	10012	00001	P 63 482 638 2	
3435 7364 4.693E-27.059D	1436.304	10012	1 0000	P 62 482 638 2	
3436 7667 5.763E-27.0600	1390,763	10012	00001	P 61 482 638 2	
3437 7919 7.050E-27.0600	1345.952	10012	00001	P 60 482 638 2	
3438 8120 8.591E-27.0600	1301.873	10012	00001	P 59 482 638 2	
3439 . 8272 1.043E+26.0610	1256.525	10012	00001	P 58 482 636 2	
3440 8373 1.261E-26.0610	1215.908	10012	00001	P 57 482 636 2	
3441 8423 1.5198-26.0610	1174.024	10012	00001	P 56 482 638 2	
3442 8424 1.6236-26.0620	1132.871	10012	00001	P 55 482 638 2	
3443 83/5 2 179E-26.0620	1092.450	10013	00001	P 54 482 638 2	
3444 4277 2.595E-26.0620	1052.761	10012	00001	P 53 482 638 2	
3445 8128 3.078E-26.0620	1013.804	10012	00001	P 52 462 638 2	
3446 0415 3 974E-27.0530	2779.506	10012	10000	P 84 482 636 2	
3446 /930 J.636E-26.0630	975.580	10 (2	00001	F 51 482 638 2	
3447 7683 4.278E-26.0630	938.089	10012	00001	P 50 402 638 2	
3448 4041 7.253E-27.0530	2649.787	10012	00001	P 82 482 636 2	
3448 7386 5.014E-26.0630	901.330	10012	00001	P 49 482 638 2	
3449 /041 5.854E-26.0640	865.304	10012	00001	P 48 482 638 2	
3450 6646 6.806E-26.0640	830.011	100 2	00001	P 47 482 638 2	
3450 7441 1.318E-26.0540	2523.146	100;2	00001	P 80 482 636 2	
345; 6202 7 882E-26.0640 3452 5709 9.091E-26.0650	795.451	10012	00001	P 46 482 638 2	
	761.625	10012	00001	P 45 482 638 2	
3453 0616 2 344E+26.0550 3453 5168 1.044E+25.0650	2399.586	10012	00001	P 78 482 636 2	
	728.532	10012	00001	P 44 482 638 2	
3454 4577 1.195E~25.0650 3455.3568 4.105E~26.0550	696,172	10012	00001	P 43 482 638 2	
3455 3936 1.361E-25.0650	2279.108 664.547	10012	00001	P 76 482 636 2	
3456 3751 1.545E-25.0660	633.655	10012	00001	P 42 482 638 2 P 41 482 638 2	
3457 . 2515 1.745E-25.0660	603.497	10012	00001		
3457 6298 7.076E-26.0560	2161.715	10012	00001		
3458 1731 1.964E-25.0660	574.072	10012	00001		
3459 0898 2.200E-25.0670	545.383	10012	00001	P 39 482 638 2 P 38 482 638 2	
3459 8808 1.201F-25.0560	2047.408	10012	00001		
3460 0018 2.455E-25.0670	517,427	10012	00001	P 72 482 636 2 P 37 482 638 2	
3460 9089 2.727E-25.067D	490.206	10012	00001	F 36 482 638 2	
3461 . 6569 3.8416-27.0620	1082.728	10012	00001	P 53 482 637 2	
3461 . 8112 3.017E-25.0680	463.719	10012	00001		
3462 1101 2.006E-25.0570	1936.190	10012	00001		
3462 . 6553 4.580E-27.0620	1042.662	10012	00001		
3462 7087 3.322E-25.0680	437.966	10012	00001		
3463 . 6014 3 . 642E-25 . 0680	412,949	10012			
3463 . 6486 5 439E-27 . 0630	1003.350	10012	00001 00001	P 33 482 638 2	
3464 . 3178 3.298E-25.0580	1826.062	10012	00001	P 51 482 637 2	
3464 4894 3 975E-25 0680	388 666	10012	00001	P 68 482 636 2	
3464 6371 0 434E-27.0630	964.791	10012	00001	P 32 482 638 2 P 50 482 637 2	
	9U7./31	14012	00001	P 50 482 617 2	

### B4. Unit 4: Output From Sample Run 2

Principal program output from Sample Run 2 is given on the following five pages.

PROGRAM NLTE FOR INFRARED RADIANCE DATE = 85/09/04. TIME = 10.13.36. TAPEI

IA---LINE DIRECTIVES

L = MOLECULE CODE x CO2
0 = 150TOPE CODE x 626
1 = UPPER VIB LVL x 10012
1 = LOWER VIB BANCH x 00001
1 = ROT'L LINE # x 14 MOL 150 UST LST BBR

18 --- VIEWING PATH PARAMETERS!

TANJ = LOWEST TANGENT HEIGHT (KM) = 70.00
TANF = HIGHEST TANGENT HEIGHT (KM) = 100.00
SPAC = EXAMINATION INTERVAL (KM) = 10.00
LOOK = 0: LOOKING GEOMETRY CHOSEN = LIMB

1C--- PROGRAM PARAMETERS:

HMAK = ASSUMED TOP OF ATL, SPHERE (KM) = 150

ACC = ACCURACY (INTEG O RADIANCE) = .01000

NPTS = HUMBER OF INTEG POINTS PER PANEL = 4

WIND = 0: LIMESHARE OPTION SELECTED = VOIGT

VMIN = LOWER END, LINE SEARCH (CM-1) = 0

VMAX = UPPER END, LINE SEARCH (CM-1) * 20000

10---SYNTHETIC SPECTRUM PARAMETERS:

FWHM = 0. SYNTHETIC SPECTRUM NOT GENERATED

1E---BAND PARAMETERS: (FOUND IN MOLPAR)

VIBE = VIB ENERGY OF THE TRANSITION (CM-1) = 3612.8420
VIBL = VIB ENERGY OF THE LOWER STATE (CM-1) = 667.3790
VIBQ = OUNNIUM FOR THE PARTITION FN (CM-1) = 667.3790

GL = STATISTICAL WEIGHT, LOWER VIBRATIONAL STATE = 1
GU = STATISTICAL WEIGHT, UPPER VIBRATIONAL STATE = 1

OUANTITIES RETURNED FROM MOLEC:

WGT = MOLECULAR WEIGHT = 44
A1 = 150TOPIC ABUND = 99414
DEGV (EXPLAINED IN MOLEC) = 2
PAOT (EXPLAINED IN MOLEC) = 1
TEXP (EXPLAINED IN MOLEC) = 1.5

FURNAT FOR THE SEARCH OF THE LINETADE IS (82.F10.4.E10.3.F5.4.F10.3.2AB.14x.A1.13.4x.14)

AD-A172 556

UPDATE OF AN EFFICIENT COMPUTER CODE (N.T.E.) TO 2/2

CALCULATE EMISSION AND TRA. (I) AR FORCE GEOPHUSICS

AFGL-TR-85-0240

P UINTERSTEINER ET AL. 7.6 3/2 85

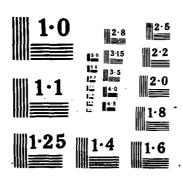
NL

END

ANT. 1000

INC. 1000

I



A1701 ATMOS PROFILE 06/10/85 AL7,TRTMP,NL,NU,ND,N1---DATA FROM VSIM, IRR---FORMERLY AT101G1, CO2MODATMOSPROF78(CV3) CO2 626 10012 00001 40-160 KM

INPUT OPTION # 4; NVP = 2, NPF = 2, VIBL = 0; (SEE COMMENTS IN ATMPR)

THE LOWER- AND UPPER-STATE POPULATIONS REFLECT AN ABUNDANCE OF .98414 W.R.T. TOTAL CO2

(1) FN	215.989 1.02387 214.485 1.02313	<u>-</u> : .	211.494 1.02169	174 1.	960 1.	376 1	-		121																			,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,																
(CM-3) (CM-3)	1,7081E+03	1.9819E+03	2.1380E+03	2.4821E+03	2.6710E+03	2.8531E+03	3.0477E+03	3.2098E+03	3.38056+03	2 ARAFFOL		3.5914E+03	3.5914E+03 3.5990E+03 3.6067E+03	3.5914E+03 3.5990E+03 3.6067E+03 3.509E+03	3,5914E+03 3,5990E+03 3,6067E+03 3,3983E+03	3.5914E+03 3.590E+03 3.509E+03 3.5009E+03 3.3983E+03 3.1676E+03	3,5914E+03 3,5906E+03 3,5009E+03 3,3983E+03 3,1676E+03 2,9526E+03	3.5914E+03 3.5990E+03 3.606F+03 3.3983E+03 3.167E+03 2.167E+03 2.6743E+03	3.5914E+03 3.5990E+03 3.5090E+03 3.3983E+03 3.3983E+03 2.952E+03 2.422E+03	3.5914E+03 3.599E+03 3.509E+03 3.509E+03 3.1676E+03 2.952E+03 2.472E+03 2.1374E+03	3.5914E+03 3.5990E+03 3.5990E+03 3.3983E+03 3.1676E+03 2.9526E+03 2.472E+03 2.1374E+03	3.59146.03 3.59906.03 3.50906.03 3.39836.03 3.16766.03 2.67436.03 2.67436.03 2.13746.03 1.88616.03	3.5914E+03 3.5990E+03 3.5090E+03 3.5099E+03 3.1676E+03 2.9526E+03 2.422E+03 2.1374E+03 1.6301E+03 1.4098E+03	3.5914E-03 3.5914E-03 3.5096E-03 3.5098E-03 3.1676E-03 2.9526E-03 2.422E-03 2.1374E-03 1.8981E-03 1.4089E-03	3.5914E+03 3.5990E+03 3.5990E+03 3.3983E+03 3.1676E+03 2.9526E+03 2.422E+03 2.1374E+03 1.6301E+03 1.1989E+03 1.1989E+03	3.5914E+03 3.5990E+03 3.5090E+03 3.5099E+03 3.5095E+03 3.1676E+03 2.422E+03 2.422E+03 1.6301E+03 1.6301E+03 1.989E+03 1.0203E+03	3.5914E+03 3.5996E+03 3.5096E+03 3.5099E+03 3.1676E+03 2.674E+03 2.674E+03 2.1374E+03 1.6861E+03 1.686E+03 1.1989E+03 1.0203E+03 8.5438E+03 5.1374E+03	3.5914E+03 3.5996E+03 3.5090E+03 3.5099E+03 3.1676E+03 2.6743E+03 2.6743E+03 2.1374E+03 1.1989E+03 1.1989E+03 1.1989E+03 1.1548E+03 1.1548E+03 1.1548E+03 1.1548E+03 1.1548E+03	3.5914E+03 3.5990E+03 3.5990E+03 3.3983E+03 3.3983E+03 2.952EE+03 2.422E+03 2.1374E+03 1.6301E+03 1.989E+03 1.1989E+03 1.2503E+03 1.2503E+03 1.2503E+03 4.9548E+02 4.9548E+02	3.5914E+03 3.5990E+03 3.5990E+03 3.5099E+03 3.1676E+03 2.674E+03 2.672E+03 2.1374E+03 1.6961E+03 1.6961E+03 1.6961E+03 1.759E+03 1.759E+03 1.759E+03 1.759E+03 1.759E+03 1.759E+03 1.759E+03	3.5914E+03 3.5996E+03 3.5096E+03 3.5099E+03 3.1676E+03 2.6745E+03 2.6745E+03 2.1374E+03 1.6861E+03 1.0203E+03 1.0203E+03 1.0203E+03 2.386E+03 3.674E+03 3.674E+03 3.674E+03 3.674E+03 3.674E+03 3.674E+03	3.59146.403 3.59966.403 3.50996.403 3.50996.403 3.16766.403 2.4276.403 2.4276.403 1.40896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403 1.10896.403	3.5914E+03 3.5990E+03 3.5090E+03 3.5099E+03 3.5099E+03 2.9526E+03 2.422E+03 2.422E+03 1.6301E+03 1.6301E+03 1.0203E+03 1.0203E+03 1.0203E+03 2.3539E+02 4.0845E+02 2.3670E+02 2.297E+02 2.297E+02	3.5914E+03 3.5990E+03 3.5990E+03 3.5990E+03 3.5099E+03 3.1676E+03 2.674E+03 2.674E+03 2.1374E+03 1.690E+03 1.690E+03 1.759E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 4.9548E+02 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	5.2972E+11 4.6006E+11	3.9956E+11	3.4482E+11	4.5611E+11	2.2043E+11	1.89196+11	1.6237E+11	1.3896E+11	1.1892E+11	1.0146E+11	-	0.400000	7.3630E+10 6.2626E+10	7.3630E+10 6.2626E+10 5.3091E+10	7.3630E+10 6.2626E+10 5.3091E+10 4.5008E+10	7.3630£+10 6.2626£+10 5.3091£+10 4.5008£+10 3.7694£+10	7.3630E+10 6.2626E+10 5.3091E+10 4.5008E+10 3.7694E+10	7.3630E+10 6.2626E+10 5.3091E+10 4.500BE+10 3.7694E+10 3.1568E+10	7.3630E+10 6.2626E+10 5.3091E+10 4.5008E+10 3.7694E+10 2.1568E+10 2.2138E+10	7.3620E+10 5.3091E+10 4.500BE+10 3.7694E+10 2.650BE+10 2.6430E+10 2.6430E+10	7.3630E + 10 5.3091E + 10 4.5008E + 10 3.1568E + 10 2.643E + 10 1.8518E + 10 1.8518E + 10	7.3630E+10 5.309E+10 4.5008E+10 3.1568E+10 3.1568E+10 2.643E+10 1.8518E+10 1.8518E+10	7.3630E+10 5.3091E+10 4.5008E+10 3.1598E+10 3.1598E+10 2.6436E+10 2.6436E+10 1.2618E+10 1.2951E+10 1.2951E+10	7.3530E + 10 5.30310E + 10 4.5030E + 10 3.7594E + 10 3.7594E + 10 2.2136E + 10 1.8513E + 10 1.8513E + 10 1.251E +	7.3630E+10 5.3091E+10 4.500BE+10 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00001 06/21/85 2.7UM REGULAR 101 COMBINATION BANDS 00001 0000 10012 LS ENERGY (CM-1) C02 626 81.9400 TMIN = TEMPERATURE USED FOR STDW = 188 STD DOPP WIDTH = STDW (CM-1) = .2675GE-O2 4-PT GAUSS QUADRATURE USED FOR NU-INTEG FREQUENCY STRENGTH WIDTH (CM-1) EXEC TIME FOR INITIALIZATION = 2.18 SEC; .074 AFGL LINE FILE FOR SELECTED TRANSITION: .396E-19 10012 3623.8933 L101000 C02 ALL BR LINE 4

GROUP # 1 WITH 4 VIEWING PATHS

O LAVERS O LAVERS O LAVERS
8555
149.00 KM 149.00 KM 149.00 KM
THRU THRU THRU
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PATH # 1. TANGENT HT # 70.00 KM, USE LAVERS 1 THRU BO (ALTITUDES 70.00 THRU 149.00 KM) BO LAVERS PATH # 2. TANGENT HT # 80.00 KM, USE LAVERS 21 THRU BO (ALTITUDES 90.00 THRU 149.00 KM) 70 LAVERS PATH # 3, TANGENT HT # 90.00 KM, USE LAVERS 21 THRU BO (ALTITUDES 90.00 THRU 149.00 KM) 60 LAVERS PATH # 4, TANGENT HT # 100.00 KM, USE LAVERS 31 THRU BO (ALTITUDES 100.00 THRU 149.00 KM) 50 LAAVERS
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ARIOUS LINE-OF-SIGHT PATHS

FREG   PRODINCE (PROPERSECTION STATES SECTION   MINIMA SUCCESSIVE INTEGRATION PARELS FOR LINE R 144, FOR CONVERSION 10 WATTER FREG   PRODINCE   TAU   MODINACE   TAU   TA	OM THE LINE CENTER) FOR VA	HCE TAU 100.00 KM	10 1.496E+00 110 1.399E+00 110 1.126E+00	90.	110 7.2226-01 110 4.846E-01 110 2.532E-01 110 1.396E-01	90.	+09 9.820E-02 +09 4.763E-02 +09 1.640E-02 +08 6.610E-03	,07	08 3.948E-03 08 1.421E-03 07 3.382E-04 06 1.053E-04	.05	.06 4.013E-05 .05 3.565E-06 .04 4.457E-07	.03	.02 .17
PROLIANE   PROLIANS CMA+STR-SEC*CM-1   AND TOTAL OPTICAL DEPTH VS FREDUENCY (CM-1 FRO INTO NO INTO N	N THE LINE 1. FOR CON	RADIANCE 100	7,3241E+10 7,1112E+10 6,3801E+10 5,4568E+10	3.54281E+08	4.8563E+10 3.6246E+10 2.1081E+10 1.2260E+10	1.56603E+08	8.7937£+09 4.3637£+09 1.5200£+09 6.1348£+08	1.90174E+07	3.6608E+08 1.3121E+08 3.0982E+07 9.5685E+06	6.32481E+05	3,6198E+06 3,1738E+05 4,1627E+04 2,7841E+04	8.04086€+03	7,9541E+02 5,7260E-17
PADIANCE   CHOTONS/CM2*518*5EC*CM*  J   AND TOTAL OPTICAL DEPTH VS FREQUENCY INTO RAD (PHOTONS/CM2*518*5EC) WITHIN SUCCESSIVE INTEGRATION PARELS FOR BOLDON KM BOLDO	COM-1 FRON	¥	9.756E+00 9.086E+00 7.203E+00 5.417E+00				5.262E-01 2.409E-01 7.580E-02 2.813E-02		1.600E-02 5.190E-03 1.062E-03 2.975E-04		1.107E-04 2.117E-05 1.254E-05 1.020E-05		
PADIANCE   PHOTONS/CM2*STR*SEC*CM-1)   AND TOTAL OPTICAL DEPTRITION RAD   PHOTONS/CM2*STR*SEC)   WITHIN SUCCESSIVE INTEGRATION	I VS FREQUENCY	RADIANCE 90.0	9.3091E+10 9.2809E+10 9.1771E+10 9.0193E+10	4.92545E+08	8.8909E+10 8.3729E+10 6.7086E+10 4.6749E+10	3.89232E+08	3.5647E+10 1.8649E+10 6.3610E+09 2.4183E+09	7.90500E+07	4 0,	2.26133E+06	9.6165E+06 1.8077E+06 1.0642E+06 8.6549E+05	2.95270E+04	2.5238E+04 1.8168E-15
FREQ	TICAL DEPTH Integratio	TAU DO KM									1.403E-03 5.482E-04 3.765E-04 3.073E-04		
FREQ	AND TOTAL OP	RADIANCE 80.0	8.80796+10 8.73076+10 8.44616+10	4.56350E+08	7.7222E+10 6.9440E+10 5.5821E+10 4.4691E+10	3.31957E+08	3.92076+10 2.85306+10 1.3760E+10 6.0742E+09	1,159106+08	3.6615E+09 1.2863E+09 2.9225E+08 9.4897E+07	6.249086+06	4.3770E+07 1.6045E+07 1.0930E+07 8.9185E+06	1.92167E+05	2.5348E+05 1.8679E-14
FREG RADIANCE (PHOTONS/CM2*STR* FREG RADIANCE 70.00.00.00.00.00.00.00.00.00.00.00.00.0	SEC CM-1)	TAU 30 KM			1.163E+02 7.928E+01 4.247E+01 2.394E+01		1,705E+01 8,486E+00 3,026E+00		7.669E-01 2.915E-01 8.227E-02 3.543E-02		2.147E-02 1.154E-02 8.166E-03 6.653E-03		
FREQ 1000186 2000883 3001792 4002469 5002861 6003558 7004467 8005164 900536 10005336 11007142 12007839 9 3 2 3 13008211 14008908 15008908 16010514 P 4 3 - 4 17011071 16012466 19014284 20015679 P 5 4 6	TONS/CM2.STR. Tons/cm2.Str.	RADIANCE 70.0	8.3575E+10 7.9916E+10 7.4763E+10	4.33487E+08	7.0989E+10 6.1805E+10 4.6308E+10 3.3438E+10	2.857726+08	2.6982E+10 1.6764E+10 8.4273E+09 4.9448E+09	7.36531E+07	3.4900E+09 1.5378E+09 4.3648E+08 1.7425E+08	6.85371E+06	9.8239E+07 4.8592E+07 3.4189E+07 2.7881E+07	5.23536E+05	8.1093E+05 5.8377E-14
PADI 1 1 1 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3	ANCE (PHO	FREQ	.000186 .000883 .001792	1 -0	.003558 .00467 .005164		.005536 .006233 .007142		.008211 .008908 .009817 .010514		.012466 .012484 .014284		CONIRIB: EC*CM2*SR /CM2*SR
	RAD1 INTD		- 2 5 4	۵	8 4 6 5		901		13		17 18 19 20		TAIL PH/S WAIT

INTEGRATED RADIANCE (WATT/(CM2"STR) FOR VARIOUS LINE-OF-SIGHT PATHS

100.00 KM 100.00 KM (THICK)	6.0958E-11 3.8192E-11
90.00 KM 90.00 KM (THICK)	3.52276-10 6.93346-11
80,00 KM 80,00 KM (THIN) (THICK)	8.0950E-10 6.5575E-11
70.00 KM 70.00 KM (THIN) (THICK)	14 8.16976-10 5.76695-11
LIME	α

# B5. Unit 5: Output From Sample Run 2

Subsidiary program output from Sample Run 2 is given on the following three pages.

PROGRAM MLTE FOR INFRARED RADIANCE DATE * 85/09/04. TIME * 10.13.38.

UAIE * 85/09/04. TIME * 10.13.36. ....... TAPES

	(SPECTRAL, AT LINE CENTER) (INTEGRATED OVER LINE)	
ALTITUDE-DEPENDENT QUANTITIES FOR LINE R 14:	VOLUME EMISSION RATE IN PHOTOMS/(SEC*CM3*CM-1*STER) (SPECTRAL, AT LINE CENTER)  R IS GIVEN IN UNITS OF PHOTOMS/(SEC*CM3*STER)  KT IS GIVEN IN UNITS OF PHOTOMS/(SEC*CM2*CM-1*STER)	S OF CM-1/MOLECULE-CM2
ALTITUDE-DEPENDENT C	NOLUME EMISSION RATE	

V.E.R.	.10936E+10	118535+10	. 12858E+10	. 13970E+10	. 15144E+10	163966+10	-	76+1	-	2E+1	-	. 23362E+10	38865+1	.24084E+10	38976+1	7	+	2094BE+1	. 19336E+10	=	-	+		. 10453E+10	50 1E	n.	3927E	33076+	363336+09	101575+0	4542E	. 19994E+09	.16307E+09	.13226E+09	567E+0	356E+0	.68963E+08	11E+0	.39887E+08	. 29664E+08	.21976E+08	. 16498E+08	.12551E+08	
VGT (0)	.16330E+03	.16389E+03	.16449E+03		.16582E+03	.16641E+03	. 16700E+03	.16760E+03	. 16820E+03	.16882E+03	.169438+03	.17006E+03	.17069E+03	.171335+03	.17198E+03	.17263E+03	.17329E+03	.17386E+03	.17447E+03	.17482E+03	. 17496E+03	.17488E+03	.17481E+03	.17474E+03	. 17457E+03	. 17430E+03	.173936+03	113485103	177576403	1675+0	. 17033E+03	.16902E+03	.16774E+03	.16610E+03	.16414E+D3	1896+0	938	699E+0	.15471E+03	. 15193E+03	.14876E+03	. 14577E+03	.14296E+03	,
HAT	.129865-02	1228E-0	6922E-0	240E-0	P	181	.54157E-03	.48365E-03	.41395E-03	.33954E-03	0	4184E	05736-0	473E	4815E	2541E-0	0609E	9682E	<b>5652E</b>	3678E	.5344BE-04	w	149E	3605	w	34376	. 10 3 2 3 5 - 0 4	7067	107165-04	.895306-05	548E	398E	.52291E-05	70 IE	6436E	03405	5242E-0	9	79E-0	ç	(E-0	05896-0	ç	17730E-0E
<u> </u>	.49635E-19	9824E-1	0014E-1	. 50203E-19	03936-1	05825-1	.507726-10	7	7	7	7	7	1916E	Z 108E-1		2488E-1	26756-1	860E-1	30026-1	31026-1	-	-	.531356-19	-	. 55094E-19	. 1375055.	01-3/257C.	5274RF-19	2643E-1	420E-1	ī	7	1400E-1	0952E-1	03976-1	973BE	89796-1	231E-1	74988-1	6578E-1	54866-1	442BE-1	406E-1	423915-19
(1-10)		_	. 28525E-02		. 48327E-02		80	. 28027E-02	.27926E-02	.27824E-02	.27723E-02	77621E-02	. 27519E-02	. 27416E-02	. 27313E-02	. 27210E-02	. 47106E-02	. 27002E-02	6922E-0	. 268695-02	6847E-0	6859E-0	. 76870E-02	0.31600	2000	70066	707F-0	71485-0	218E-0	.27362E-02	o	.27791E-02	. ZB003E-02	. 28279E-02	7/10	.29015E-02	34/15	. 299 20t - UZ	.30352E-02	.309165-02	.31576E-02	7.23E-0	2857E-	.33496F-02
:	280E+1	2578E+1	40545E+10	10000	011110000		0021241	12268E+11	1736+1	9662E+1	740E	7456E+	32/325+11		1447336411	. 5 1 188E • 11		704775411	10.77.01.	. /614/E+11	01322E+11	6050505	11.306669.	049806411	966186+11	7653F	98066E+11	.98037E+11	.97567E+11	.96789E+11	S	.94510E+11	932045+11	91080E+11		, ,	. 00 134C+11	10010	- ר	76.495.4	45/2E	37875	3574E	83149E+11
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172E+00 1746E+00 1136F+00 9164E-01 5977E-01 5977E-01 3196E-01 2538E-01		0.00
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659E 10 6 0E 10 5 0E 10 5 0E 10 4 39E 10 3 77E 10 3 2 2 2 10 1 8 2 E 10 1 1 9 E 10	975E 09 678E 09 480E 09 235E 09 193E 09 193E 09 480E 08 236E 08	2446.07 2046.07 2046.07 1536.07 1316.07 1316.07 1456.06 6556.06 6556.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.06 6572.0
1819E+00 1324E+00 8083E+00 7234E-01 5897E-01 3943E-01 3943E-01 2500E-01 211E-01 211E-01 233E-01	11766 01 90636 02 41996 02 31146 02 2296 02 2296 02 12996 02 12996 03 12996 03 12996 03 12996 03 12996 03 12996 03 12996 03 12996 03 16976	
11 26 11 29 11 29 11 20 20 20 20 20 20 20 20 20 20 20 20 20	99999999999999999999999999999999999999	7 7 7 7 7 7 7 7 8 8 9 9 9 9 9 9 9 9 9 9
99.2 99.2 99.0 99.0 99.0 99.0 100.0 101.0	100 5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	130.0 132.0 133.0 133.0 133.0 135.0 135.0 135.0 135.0 141.0 141.0 141.0 141.0 141.0 141.0

## B6. Unit 6: Output From Sample Run 2

Diagnostic output from Sample Run 2 is given on the next page.

		(FORWAT) (DATA)	(HEADER) (HEADEP) (HEADER) (FORMAT) (DATA)	(MEADER) (MEADER) (COPMAT) (DATA)
PRUJRAM 11, "OR INFRARED RADIANCE UATE = 85/L_/04, TIME = 10.13.36. TAPES	PRINT THE MEADERS AND FIRST DATA CARD-IMAGES FOUND ON INPUT UNITS	UNIT 1: 111111111122222222233333333444444444444	UNIT 2: CA1701 ATMOS PROFILE 06/10/85 CA1701 ATMOS PROFILE 06/10/85 CA1701 ATMOS PROFILE 06/10/85 CA1701 ATMOS PROFILE 06/10/85 CA171 TRYMP, HALVING WAS ATMOSTED WAS ATMOSTED	.mtl J. (02 ALL 10012 00001 06/21/85 2.7UM REGULAR 101 COMBINATION BANDS 101 00001 10011 00001 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 10010 1

## Appendix C

NLTE Program and Subroutine Listings

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```
PROGRAM NLTE
C
Ċ
C
                               PROGRAM NLTE
Ċ
              PREPARED FOR AIR FORCE GEOPHYSICS LABORATORY
C
                          HANSCOM AFB, MA, 01730
                                    ΒY
00000000
                          PETER P. WINTERSTEINER
                            ARCON CORPORATION
                            260 BEAR HILL RD.
                            WALTHAM, MA, 02154
C
      *************************
      PROGRAM NLTE: LINE-BY-LINE CALCULATION OF INFRARED AIRGLOW FROM
C
      NON-LTE REGIONS OF THE ATMOSPHERE. COMPONENT OF A.F.G.L. ATMOS-
000
      PHERIC RADIANCE CODE (ARC).
C
      ********
      REAL KT, INU, NU, EXPL
      INTEGER RQL, DNU, PFAC, DIML
      LOGICAL CMPL, FLAG
      PARAMETER (DIML=500, CMPL=.FALSE., EXPL=674.)
      CHARACTER*2 BR(DIML), BL
      CHARACTER*24 AST
      DIMENSION ALT(250), TRTMP(250), ALCOR(250), RHO(250), TVL(250)
      DIMENSION QRAT(250), ZZ(250,5), R(250), DWID(250), VGT(250)
      DIMENSION KT(250), TVU(250), STORE(DIML, 5), CUM(250)
      DIMENSION RAT(250), HGTS(50)
      DIMENSION V(DIML), STS(DIML), ALF(DIML), EDP(DIML), RQL(DIML)
      DIMENSION RAD(5), RAW(5), SUMRD(5), SUMPH(5), HTS(5), THR(5), TOD(5)
      DIMENSION SUM(5), K1(5), KM(5), TRN(5), LMAX(5)
      DIMENSION INU(8,5), OD(8,5), CC(8), W(4), C4(2), C8(4), W4(2), W8(4)
      DIMENSION NU(8)
      EQUIVALENCE (V(1), STORE(1,1))
C
      COMMON/A/ALT, TRTMP, ALCOR, RHO, TVL, TVU, QRAT, ZZ, KT,
               KMAX,C2,BST,TMIN
      COMMON/B/V, STS, ALF, EDP, RQL, NRL, HGTS, ACC, NPTS, NDP,
               WGT, LOOK, NREPS, IMXX, JMAX, FWHM
     1
      COMMON/C/RAT, DWID, VGT
С
      DATA FLAG/.FALSE./
      DATA (C4(I), I=1,2)/.43056815579703, .16999052179243/
      DATA (W4(I),I=1,2)/.17392742256873, .32607257743127/
DATA (C8(I),I=1,4)/.48014492824877, .39833323870681, .26276620495816, .091717321247825/
      DATA (W8(I), I=1,4)/.050614268145188, .11119051722669,
                          .15685332293894, .18134189168918/
C
  100 FORMAT(//)
  101 FORMAT(1X)
  103 FORMAT(/, EXEC TIME FOR INITIALIZATION = ', F6.2, ' SEC; ', 17,
     1' LINES',//)
```

```
104 FORMAT(///,' RADIANCE (PHOTONS/CM2*STR*SEC*CM-1) AND TOTAL',
     1' OPTICAL DEPTH VS FREQUENCY (CM-1 FROM THE LINE CENTER)',
     2' FOR VARIOUS LINE-OF-SIGHT PATHS',/,
        INTD RAD (PHOTONS/CM2*STR*SEC) WITHIN SUCCESSIVE INTEGRATION',
     4' PANELS FOR LINE ',A2,I4,
     5'. FOR CONVERSION TO WATTS, MULTIPLY BY', Ell.5,
     6//,8X,'FREQ ',5(A1,3X,'RADIANCE',5X,'TAU',3X))
  105 FORMAT(I4,F9.6,1P,5(E13.4,E10.3))
  106 FORMAT(3X,'ALT',8X,'R',9X,'DWID',9X,'KT',10X,'RAT',7X,'VGT(0)',
16X,'V.E.R.',/,3X,'(KM)',16X,'(CM-1)',31X,'(CM)',/)
  107 FORMAT(1X,F6.2,6E12.5)
  108 FORMAT(//,' OPTICAL DEPTHS (LINE CENTER) GEOMETRICAL DIS',
     1'TANCES (KM) AND RADIANCE CONTRIBUTIONS (PH/SEC*CM2*SR*CM-1',
     2' AT LINE CENTER) FOR EACH LAYER',//,
     33X,'ALT',5(Al,' DIS',5X,'O.D.',6X,'RAD',2X))
  109 FORMAT(1X,F5.1,5(F7.2,E10.4,E9.3))
  110 FORMAT(1X, 'TOTAL', 5(E17.4, E9.3))
  111 FORMAT(1X,A2,I5,1P,5(1X,E11.4,12X))
  112 FORMAT(1H+,6X,1P,5(13X,E11.4))
113 FORMAT(/,' INTEGRATED RADIANCE (WATT/(CM2*STR) FOR VARIOUS LINE',
  1'-OF-SIGHT PATHS',//,1X,'LINE',2X,5(F10.2,' KM',F8.2,' KM'))
114 FORMAT(3X,'TIME',7X,'LB',5(A1,'LL KM RADIANCE OP DPTH'))
  115 FORMAT(//,'
                    CUMULATIVE INTEGRATED RADIANCE (WATT/CM2*STR) AND '
     1'TOTAL OPTICAL DEPTH (AT LINE CENTER) FOR VARIOUS LINE-OF-SIGHT ',
     2'PATHS',//,3X,'EXEC LINE',5X,4(Fll.2,' KM',10X),Fll.2,'KM')
  116 FORMAT(1X,F6.2,1X,A2,2I3,5(2)
  117 FORMAT(//, TOTAL BAND RAP
  118 FORMAT(/,I5,' LINES',/,I5,' THICK',/)
  119 FORMAT(/,3X,'WATT/(CM2*STR): ',1P,4(E11.4,13X),E11.4)
  120 FORMAT(' PH/(SEC*CM2*STR): ',1P,4(E11.4,13X),E11.4)
121 FORMAT(11X,5(A1,'(THIN)',5X,'(THICK)',5X))
  122 FORMAT(/, 'TMIN = TEMPERATURE USED FOR STDW = ', 14,
     1/,' STD DOPP WIDTH = STDW (CM-1) =',Ell.5,
     2/,I2,'-PT GAUSS QUADRATURE USED FOR NU-INTEG')
  123 FORMAT(' WATT/CM2*SR ',1P,5(E12.4,11X))
  124 FORMAT(12X,5(F16.2,' KM',4X))
125 FORMAT(/,' TAIL CONTRIB:',/,' PH/SEC*CM2*SR',1P,5(E12.4,11X))
  126 FORMAT(/,' P',I2,I5,'-',I3,1P,5(E13.5,10X))
  127 FORMAT(' $$$$$ CAUTION: LINE ',A2,I4,' IS VERY THICK, TOD(0) ='.
     1E9.3, 'FOR', F7.2, 'KM PATH, TAIL APPROXIMATION MAY BE IN ERROR',
     2' $$$$$')
  128 FORMAT(//,' ALTITUDE-DEPENDENT QUANTITIES FOR LINE ',A2,I4,':',//,
     1' VOLUME EMISSION RATE IN PHOTONS/(SEC*CM3*CM-1*STER) (SPECTRAL',
     2', AT LINE CENTER)',/,21X,
     3' OR PHOTONS/(SEC*CM3*STER)
                                              (INTEGRATED OVER LINE)',/,
     4' R IS GIVEN IN UNITS OF PHOTONS/(SEC*CM2*CM-1*STER)',/,
     5' KT IS GIVEN IN UNITS OF CM-1/MOLECULE-CM2',//)
  129 FORMAT(' ******',5(A24))
  130 FORMAT(//,' $$$$ CAUTION---BECAUSE JMAX >',14,', NLTE CANNOT',
     1' HANDLE MORE THAN 5 VIEWING PATHS IN ONE RUN.',/,17X, 'RERUN'
     2' NLTE TO HANDLE THE HIGHER-ALTITUDE PATHS $$$$$',//)
  990 FORMAT(///,' ***** REQUESTED LINES NOT FOUND *****',///)
      **********
C
C
      PARAMETER STATEMENTS APPEAR IN NLTE, LINES, AND SPECTRM. THEY SHOULD
      BE MADE CONSISTENT WITH EACH OTHER. THE PURPOSE OF CMPL IS TO PRO-
C
      VIDE AN OPTION TO LIST LIMITED PROGRAM OUTPUT TO UNIT 9, WHICH IS E-
C
      QUIVALENT TO OUTPUT. THIS IS FOR USE IN INTERACTIVE PROCESSING AND
      IS INVOKED BY INCLUDING THE DS PARAMETER ON THE FTN5 CONTROL CARD.
```

```
AT THIS POINT THE DATA HAVE ALL BEEN READ IN AND STORED IN THE PROPER
С
C
      ARRAYS. NOW DO SOME FURTHER INITIALIZATION AND THEN PROCEED WITH THE
      LOOPS WHICH PERFORM THE ACTUAL CALCULATIONS.
С
      STDW IS THE STANDARD DOPPLER WIDTH WHICH IS USED TO DEFINE PANELS FOR
С
      THE NU-INTEGRATION. THE CC DEFINE THE INTEGRATION POINTS, AND THE W'S
C
      ARE THE WEIGHTS. NPTS (WHICH CAN BE 2, 4, OR 8) IS THE NUMBER OF IN-
С
      TEGRATION POINTS PER PANEL.
C
C
C
      IF(JMAX.EQ.0)GO TO 998
      DOPP = A2*SQRT(2.0*BOLTZ*C2/(WGT*C*C))
      STDW = DOPP*SQRT(TMIN/C2)*VIBE
      IF (NPTS.EQ.2) THEN
          CC(1) = -.288675134595*STDW
          CC(2) = -CC(1)
          W(1) = .50
      ELSE IF (NPTS.EQ.4) THEN
          DO 202 I = 1,2
          CC(I) = -C4(I)*STDW
          CC(5-I) = C4(I)*STDW
                = W4(I)
  202
         W(I)
      ELSE
          DO 203 I = 1.4
          CC(I) = -C8(I)*STDW
          CC(9-I) = C8(I)*STDW
                = W8(I)
  203
          W(I)
      END IF
      I = TMIN
      WRITE(4,122)I,STDW,NPTS
      THE TOTAL NUMBER OF DIFFERENT LINE-OF-SIGHT PATHS TO BE CONSIDERED
      IN ALL IS IMX, (FIXED IN LINES).
С
                                         THESE CASES ARE DONE IN GROUPS OF
      FIVE (POSSIBLY LESS, IN THE CASE OF THE LAST GROUP) IN ORDER TO MAKE
С
      THE PRINTED OUTPUT MANAGEABLE AND ALSO TO REDUCE THE SIZE OF CERTAIN
C
      ARRAYS. THE LOOP DO 500 IS ENTERED ONCE FOR EACH GROUP. THE ARRAY
C
      HGTS STORES THE HEIGHTS (IN KM) WHICH PARAMETERIZE EACH PATH. NREPS
      (ALSO FIXED IN LINES) IS THE NUMBER OF GROUPS WHICH MUST BE HANDLED.
C
С
      NOTE THAT IF THERE ARE MORE THAN 500 LINES IN THE BAND UNDER CONSI-
C
      DERATION ONLY 5 VIEWING PATHS CAN BE PROCESSED IN ONE RUN.
С
С
      TS = SECOND() - TZ
      WRITE(4,103)TS,JMAX
C$
      IF(CMPL)
      WRITE(9,103)TS, JMAX
C$
      ENDIF
      IF (JMAX.GT.DIML) THEN
          JMAX = DIML
          IF (NREPS.GT.1) THEN
              NREPS = 1
              WRITE(4,130)DIML
              WRITE(6,130)DIML
          END IF
      END IF
```

```
C*
      LOOP TO SELECT GROUPS OF (5 OR LESS) LINE-OF-SIGHT PATHS. CALCULATE
C*
      THESE CASES ALL AT ONCE. WHEN THIS LOOP ENDS, EXECUTION TERMINATES.
C*
C*
      SUBROUTINE PATH RETURNS IMAX, THE NUMBER OF PATHS IN THE GROUP SPE-
      CIFIED BY THE INDEX NR AND STACKS IMAX VALUES OF HGTS INTO THE VEC-
C*
      TOR HTS. IT ALSO DETERMINES THE LOWER-ALTITUDE INDEX, K1, FOR EACH
C*
C*
     PATH.
C*
      DO 500 NR = 1, NREPS
     LCNT = 1
      JCNT = 0
     IF(JMAX.EQ.1)FLAG = .TRUE.
      CALL PATH(ALT, HGTS, IMXX, HTS, IMAX, NR, KMAX, LOOK, K1)
      SUMRD AND SUMPH ARE ARRAYS THAT STORE THE SUM OF RADIANCES FROM RO-
C*
      TATIONAL TRANSITIONS FOR THE 1TH LINE-OF-SIGHT PATH.
                                                          PRESET THESE
C*
C*
      ARRAYS TO ZERO. ALSO CALCULATE THE ARRAY OF PATH LENGTHS, ZZ, FOR
      EACH LAYER (K) AND EACH PATH (I) IN THIS GROUP. THE FACTOR 10**5
      CONVERTS KM TO CM, AND THE FACTOR RHO(K) CONVERTS ZZ TO THE COLUMN
C*
C*
     DENSITY.
     DO 220 I = 1,IMAX
      SUMPH(I) = 0.0
      SUMRD(I) = 0.0
     DO 220 K = Kl(I), KMAX
      IF (LOOK.EQ.1) THEN
         Z2 = ALT(K+1) - ALT(K)
         IF(K.EQ.Kl(I))ZZ = ALT(K+1) - HTS(I)
      ELSE
         Z1 = ALT(K) - HTS(I)
         IF(Z1.LT.0.0)Z1 = 0.0
         Z1 = SQRT(Z1*(2.0*EARTHR + ALT(K) + HTS(I)))
         Z2 = SQRT((ALT(K+1)-HTS(I))*(2.0*EARTHR+ALT(K+1)+HTS(I))) - Z1
      END IF
  220 ZZ(K,I) = RHO(K)*Z2*1.0E+05
      IF (FLAG. AND. NR. EQ. 1) THEN
         WRITE(5,128)BR(1),RQL(1)
         WRITE(5,106)
      END IF
C**
C**
      LOOP TO PERFORM CALCULATIONS ON ALL THE ROTATIONAL LINES SELECTED.
C**
      LINES ARE READ FROM TAPE3 IN BATCHES OF 500, MAXIMUM. IF THERE ARE
C**
      MORE THAN 500 LINES ON THE LINEFILE THIS LOOP IS ENTERED MORE THAN
C**
      ONCE. (SYMBOLIC CONSTANT DIML IS SET TO 500 FOR THIS PURPOSE.) IF
C**
      THERE ARE MORE THAN 500 LINES, A MAXIMUM OF FIVE L-O-S PATHS CAN
C**
      BE RUN.
C**
C**
      OO CORRECTS FOR THE STIMULATED EMISSION AT TS (296 K).
C**
  225 DO 400 J = 1, JMAX
      VINIT = V(J)
      ALFL = ALF(J)
      QQ = 1.0 - EXP(-VINIT/BST)
C * *
C**
            C** *
C** * THE LOOP DO 230 CALCULATES THOSE PATH-INDEPENDENT QUANTITIES WHICH
```

```
C** * DEPEND ONLY ON ALTITUDE. ALTITUDES RUN FROM THE LOWEST REQUIRED
C * * FOR THE FIRST (LOWEST) LINE-OF-SIGHT PATH TO THE HIGHEST REQUIRED
 * * FOR THE LAST PATH IN THE CURRENT GROUP.
  * * GAM = (GL*NU)/(GU*NL)
             SIMILAR TO NOTATION IN BULLITT ET AL, JQSRT (T.B.P., 1985)
  * * DWID = DOPPLER WIDTH (CM-1)
 * * RAT = LORENTZ TO DOPPLER LINEWIDTH RATIO FOR THE VOIGT FUNCTION
           = CORRECTED LINE STRENGTH. QRAT*EXP(ARG) IS JUST THE RATIO
С
             PL(TVL,T)/PL(TS,TS) WHERE PL(T1,T2) IS THE PROBABILITY THAT
C
             THE LOWER RO-VIB STATE IS OCCUPIED AT THE VIBRATIONAL TEMP-
             ERATURE T1 AND THE ROTATIONAL TEMPERATURE T2.
C
C
      DO 230 K = K1(1), KMAX
      ARG = (VIBE-VINIT)/TRTMP(K) - (VIBL+VIBE)/TVU(K) + VIBL/TVL(K)
      GAM = EXP(ARG)
      R(K) = (GAM/(1.0-GAM))*2.0*C*VINIT*VINIT
      ARG = EDP(J)/BST - (EDP(J)-VIBL)/TRTMP(K) - VIBL/TVL(K)
      KT(K) = STS(J)*QRAT(K)*(1.0 - GAM)*EXP(ARG)/QQ
      DWID(K) = DOPP*SQRT(TRTMP(K))*VINIT
  230 RAT(K) = A2*ALFL*ALCOR(K)/DWID(K)
      DV = 0.0
      IF(NDP.LT.0)THEN
          DO 231 K = Kl(1), KMAX
  231
          VGT(K) = VWERF(DV, RAT(K))/DWID(K)
      FLSE
          CALL ZVGTC(DV, K1(1), KMAX)
      END IF
С
      IF(FLAG.AND.NR.EQ.1)THEN
          DO 232 K = Kl(1), KMAX
          TAU = KT(K)*VGT(K)*RHO(K)*1.0E+05*R(K)
          WRITE(5,107)ALT(K),R(K),DWID(K),KT(K),RAT(K),VGT(K),TAU
     END IF
C
  * * THE LOOP DO 240 I=1, IMAX CALCULATES THE RADIANCE, THR, FOR EACH PATH
  * * ON THE ASSUMPTION THAT THE LINE IS "THIN". IT ALSO CALCULATES THE TO-
  * * TAL OPTICAL DEPTH AT THE LINE CENTER, AND THEN DECIDES WHETHER TO GO
     THROUGH THE "THICK" CALCULATION ON THE BASIS OF ITS VALUE.
                                                                   INUM IS
  * * THE NUMBER OF PATHS IN THE CURRENT GROUP FOR WHICH TO DO THE "THICK"
  * * CALCULATION. ALSO, FOR EACH PATH, THE ARRAY TRN USED TO EVALUATE THE
 * * TAIL OF THE RADIANCE PROFILES IS CALCULATED. LBND AND LMAX ARE INDI-
  * * CES SPECIFYING THE INTEGRATION PANELS AT WHICH THE PANEL-WIDTH IS
  * * FIRST AUGMENTED AND AFTER WHICH THE NUMERICAL INTEGRATION IS CUT OFF,
  * * RESPECTIVELY. ALSO, INITIALIZE THE RADIANCE ARRAYS WITH THE THIN-LINE
 * * RESULTS, AND CHOOSE KM(I), THE MAXIMUM ALTITUDE NEEDED FOR THE ITH
С
 * * VIEWING PATH.
      INUM = 0
      KLAR = 0
      LBND = 0
      MTAU = 1
      DO 240 I = 1,IMAX
      LMAX(I) = 0
      TOD(I) = 0.0
```

```
THR(I) = 0.0
    TRN(I) = 0.0
    SUM(I) = 0.0
    KM(I) = KMAX
    IF (LOOK. EQ. 0) THEN
        KI = KMAX
        KF = Kl(I)
        KD = -1
    ELSE
        KI = Kl(I)
        KF = KMAX
        KD = 1
    END IF
    QK = 1.0
    DO 235 K = KI, KF, KD
      TAU = KT(K)*22(K,I)
      THR(I) = THR(I) + R(K)*TAU
      TRN(I) = TRN(I) + R(K)*TAU*ALCOR(K)*ALFL
      TAU = TAU*VGT(K)
      TOD(I) = TOD(I) + TAU
      IF(TOD(I).LE.EXPL)THEN
          EK = EXP(-TAU)
          Z2 = QK*(1.0 - EK)*R(K)
          SUM(I) = SUM(I) + Z2
          CUM(K) = SUM(I)
          QK = QK *EK
      ELSE
          Z2 = EXP(-EXPL)
          CUM(K) = 0.0
      END IF
      IF(FLAG)THEN
          L = K - Kl(1) + 2
          STORE(L,I) = TAU
          STORE(L+KMAX,I) = Z2
      END IF
235 CONTINUE
    IF(NDP.EQ.1)THEN
        TRN(I) = THR(I)*DWID(Kl(I))/(A2*SQRT(PI))
        TRN(I) = TRN(I)*2.0/PI
    END IF
    IF(LOOK.EQ.0)THEN
        THR(I) = 2.0*THR(I)

TOD(I) = 2.0*TOD(I)
        TRN(I) = 2.0*TRN(I)
    END IF
    RAD(I) = THR(I)
    THR(I) = THR(I)*H*C*VINIT
    RAW(I) = THR(I)
    IF(TOD(I).GT.TOD(MTAU))MTAU = I
    IF(TOD(I).GT.(3.0*ACC).OR.FLAG)THEN
        INUM = I
       RAD(I) = 0.0
        IF(LOOK.EQ.0)THEN
            Z2 = SUM(I)*ACC
            DO 238 K = KMAX,Kl(I),-1
            IF(CUM(K).GT.Z2)GO TO 240
            KM(I) = K
238
            CONTINUE
       ELSE
```

```
Z2 = (1.0 - ACC)*SUM(I)
               DO 239 K = KMAX, Kl(I), -1
               IF(CUM(K).LT.Z2)GO TO 240
  239
               KM(I) = K
          END IF
      END IF
  240 IF(KLAR.LT.KM(I))KLAR = KM(I)
C
C
 * * IF THERE IS ONLY ONE LINE UNDER CONSIDERATION....
С
          WRITE SOME INFORMATION TO TAPE5
          WRITE A HEADER TO TAPE4
RESET INUM SO THE "THICK" CALCULATION IS PERFORMED REGARDLESS OF
  * *
C
C
          THE OPTICAL DEPTH
      IF (FLAG) THEN
          INUM = IMAX
          ARG = H*C*VINIT
          WRITE(4,104)BR(1), RQL(1), ARG, (BL, I=1, INUM)
          WRITE(4,124)(HTS(I), I=1, INUM)
          WRITE(4,101)
          WRITE(5,108)(BL, I=1, IMAX)
          WRITE(5,101)
          DO 245 K = Kl(1), KMAX
          L = K - Kl(1) + 2
          DO 244 I = 1,IMAX
          IF((Kl(I)-Kl(1)+2).GT.L)GO TO 244
          LL = I
          CUM(I) = 1.0E-05*ZZ(K,I)/RHO(K)
          CONTINUE
  244
          WRITE(5,109)ALT(K),(CUM(I),STORE(L,I),STORE(L+KMAX,I),I=1,LL)
  245
          WRITE(5,101)
          WRITE(5,110)(TOD(I),SUM(I),I=1,IMAX)
С
С
      SET ICUR, THE NUMBER OF PATHS PRESENTLY UNDER CONSIDERATION FOR THE
С
      "THICK" CALCULATION. INITIALIZE THE PANEL-WIDTH FACTOR, PFAC (INTE-
      GER) AND THE NU-INDEX, DNU (INTEGER). (DNU GIVES THE NUMBER OF STAN-
C
      DARD DOPPLER WIDTHS FROM THE LINE-CENTER TO THE END OF THE CURRENT
C
      INTEGRATION PANEL.) JCNT IS THE NUMBER OF "THICK" LINES ENCOUNTERED.
С
      IF(INUM.EQ.0)GO TO 360
      JCNT = JCNT + 1
      PFAC = 1
      DNU = 0
      ICUR = INUM
C *
C
      THE LOOP DO 350 LL = 1,50 SELECTS THE PANELS (OF WIDTH STDW*PFAC)
C
      WITHIN WHICH TO PERFORM NPTS-PT GAUSS-LEGENDRE QUADRATURE OVER FREQU-
С
      ENCY. THE LOOP DO 300 L = 1, NPTS EVALUATES THE INTEGRAND AT THE NPTS
      CHOSEN FREQUENCIES FOR EACH L-O-S PATH, AND THE INTEGRALS THEMSELVES ARE EVALUATED AT STATEMENT 305. THE INTEGRAND IS THE RADIANCE INTE-
```

```
GRATED ALONG THE L-O-S PATH---THAT IS THE INTEGRAL OVER Z. THIS Z-IN-
C **
      TEGRATION IS THEREFORE CARRIED OUT COMPLETELY FOR THE FIRST OF THE
C **
      NPTS POINTS (THE FIRST FREQUENCY) FOR ALL L-O-S PATHS BEFORE THE SE-
C **
      COND IS CONSIDERED.
С
  * *
      FOR LIMB-LOOK, THE Z-INTEGRATION IS DONE IN TWO PIECES (LOOPS ENDING
C
  * *
 * *
С
      AT 260 AND 265). FOR ZENITH-LOOK, ONLY THE SECOND PIECE IS REQUIRED.
  * *
С
C **
      DO 350 LL = 1.50
C **
      DNU = DNU + PFAC
      CPAN = STDW*DNU - STDW*PFAC/2.0
      DO 300 L = 1.NPTS
        DV = CPAN + CC(L)*PFAC
С
 ** *********************
C ***
C ***
        LINESHAPE:
                        CALCULATE, FOR ALL ALTITUDES REQUIRED, THE VALUES
C ***
        OF THE VOIGT PROFILE AT THE "DISTANCE" FROM THE CENTER OF THE LINE
        DETERMINED BY THE CURRENT VALUES OF L AND LL---THAT IS, DV CM-1
 ***
C
 ***
        FROM THE CENTER. THE DOPPLER OPTION IS INCLUDED IN ZVGTC. RESULTS
С
C ***
        ARE STORED IN ARRAY VGT.
C ***
        IF(NDP.LT.0)THEN
            DO 251 K = Kl(1), KLAR
            Z2 = DV/DWID(K)
  251
            VGT(K) = VWERF(Z2,RAT(K))/DWID(K)
            CALL ZVGTC(DV, K1(1), KLAR)
        END IF
C ***
C ** *
C **
C ** *
C ***
 ***
С
        THE LOOP DO 270 I = 1,ICUR SELECTS DIFFERENT LINE-OF-SIGHT PATHS.
C ***
        SUM IS (TEMPORARILY) THE OPTICAL DEPTH ALONG THE PATH AT THE CUR-
C ***
        RENT FREQUENCY. INU (REAL) IS THE RADIANCE.
C ***
        DG 270 I = 1,ICUR
           SUM(I) = 0.0
           INU(L,I) = 0.0
C ***
C ***
           START THE Z-INTEGRATION ALONG THE LINE-OF-SIGHT AT THE TOP OF
C ***
           THE ATMOSPHERE. THE LOOP DO 260 CARRIES THE CALCULATION FROM
C ***
           THE OBSERVER TO THE TANGENT POINT FOR LIMB-LOOK GEOMETRY. THIS
C ***
           LOOP IS BYPASSED FOR ZENITH-LOOK.
C ***
           QK = 1.0
           IF(LOOK.EQ.1)GO TO 263
           DO 260 K = KM(I), Kl(I), -1
               TAU = KT(K)*ZZ(K,I)*VGT(K)
               SUM(I) = SUM(I) + TAU
               IF(SUM(I).GT.EXPL)GO TO 260
               EK = EXP(-TAU)
               INU(L,I) = INU(L,I) + QK*(1.0 - EK)*R(K)
               OK = OK * EK
 260
           CONTINUE
           IF(SUM(I).LT.EXPL)GO TO 263
```

```
SUM(I) = 2.0*SUM(I)
            GO TO 268
C ***
C ***
            FOR LIMB-LOOK, COMPLETE THE Z-INTEGRATION BY CARRYING IT FROM
C ***
            THE TANGENT POINT THROUGH ALL SLABS TO THE FAR HORIZON. FOR ZENITH-LOOK THIS LOOP DOES THE COMPLETE CALCULATION FROM THE
 **
C
C ***
            THE OBSERVER TO TOP OF THE ATMOSPHERE.
C ***
  263
            DO 265 K = Kl(I), KM(I)
                 TAU = KT(K)*ZZ(K,I)*VGT(K)
                 SUM(I) = SUM(I) + TAU
                 IF(SUM(I).GT.EXPL)GO TO 265
                 EK = EXP(-TAU)
                 INU(L,I) = INU(L,I) + QK*(1.0 - EK)*R(K)
                 QK = QK*EK
             CONTINUE
  265
  268
             NU(L) = DV
            OD(L,I) = SUM(I)
  270
        CONTINUE
 ***
 **
С
C **
  300 CONTINUE
C **
C **
      PERFORM 2-, 4-, OR 8-PT GAUSSIAN INTEGRATION OVER THE CURRENT PANEL,
C **
      AND ADD THE RESULT TO THE ACCUMULATING SUMS STORED IN RAD.
 **
C
      TAU = SUM(MTAU)
      DO 310 I = 1, ICUR
      LMAX(I) = LL
      SUM(I) = 0.0
      DO 305 K = 1,NPTS/2
  305 SUM(I) = SUM(I) + W(K)*(INU(K,I) + INU(NPTS+1-K,I))
      SUM(I) = 2.0*SUM(I)*STDW*PFAC
  310 RAD(I) = RAD(I) + SUM(I)
C **
C **
      IF THERE IS ONLY ONE LINE, PRINT THE LINESHAPE AND THE RESULTS OF THE
C **
      INTEGRATION OVER SUCCESSIVE PANELS AS THEY ARE PROCESSED.
C
 * *
      IF (FLAG) THEN
          DO 320 L = 1, NPTS
          K = (LL-1)*NPTS + L
  320
          WRITE(4,105)K,NU(L),(INU(L,I),OD(L,I),I=1,ICUR)
          K = DNU - PFAC
          WRITE(4,126)LL,K,DNU,(SUM(I),I=1,ICUR)
          WRITE(4,101)
      END IF
C **
C **
      CHECK TO SEE IF THE NUMERICAL INTEGRATION CAN BE CUT OFF. IF SO, ADD
C **
      IN THE ANALYTICAL RESULT FOR THE TAIL AND DECREMENT ICUR. SKIP OUT
C **
      OF THE FREQUENCY LOOPS IF ALL PROFILES ARE CUT OFF.
C **
      IF(DNU.GE.5) THEN
          L = 0
          DO 330 I = ICUR, 1, -1
          21 = 1.0
          IF(NDP.EQ.1)THEN
               Z1 = DNU*STDW*A2/DWID(K1(I))
               21 = EXP(-21*21)
          END IF
```

```
S = Z1*TRN(I)/(DNU*STDW)
         Z2 = 6.0*ACC*RAD(I)/OD(NPTS,I)
          IF(S.LT.Z2)THEN
             L = L + 1
              TRN(I) = S*(1. + (DWID(K1,I))/(DNU*STDW))**2/(2.*A2*A2))
             IF(NDP.EQ.1)TRN(I) = S
             RAD(I) = RAD(I) + TRN(I)
  330
         CONTINUE
         ICUR = ICUR - L
      END IF
      IF(ICUR.LE.0)GO TO 360
C **
     CHECK TO SEE IF THE PANEL WIDTH CAN BE EXPANDED TO PERFORM THE NUMER-
C **
C **
      ICAL INTEGRATION IN THE TAIL MORE QUICKLY. THE PATH WITH THE GREATEST
C **
     OPTICAL DEPTH TRIGGERS THE EXPANSION FOR ALL PATHS.
C **
      IF(LL.GE.3.AND.TAU.LT..5)THEN
          IF(LBND.EQ.0)LBND = LL
          IF(PFAC.LT.500)PFAC = 2*PFAC
      END IF
  350 CONTINUE
C **
C **
     END THE LOOP (INDEX LL) THAT SELECTS THE INTEGRATION PANELS. THE
C **
     INTEGRATION IS NOW COMPLETE FOR ALL L-O-S PATHS FOR THE PRESENT LINE,
C **
     EXCEPT POSSIBLY FOR THE TAIL CONTRIBUTION, ADDED IN AT STATEMENT 355
     FOR THE MOST EXTREME THICK-LINE CASES. (NORMALLY, EXECUTION WILL SKIP
 * *
     OUT OF THE LOOP DO 350 TO STATEMENT 360. IF THE LINE IS SO EXTREMELY
C **
     THICK THAT THE PANEL-EXPANSION PROCEDURE HAS NOT EVEN BEEN INVOKED,
     A DIAGNOSTIC MESSAGE IS WRITTEN TO UNIT 6 BECAUSE THE APPROXIMATION
     FOR THE TAIL CONTRIBUTION MAY BE IN ERROR. GENERALLY THE 50-PANEL
     RANGE OF THE LOOP DO 350 IS SUFFICIENT TO AVOID THIS DIFFICULTY.)
C * *************
C *
      S = DNU*STDW
      DO 355 I = 1,ICUR
      IF (NDP.EQ.1) THEN
         Z1 = S*A2/DWID(K1(I))
         TRN(I) = EXP(-Z1*Z1)*TRN(I)/S
         TRN(I) = (TRN(I)/S)*(1.0 + (DWID(K1(I))/S)**2/(2 - A2*A2))
      END IF
  355 RLD(I) = RAD(I) + TRN(I)
      IF(PFAC.EQ.1)WRITE(6,127)BR(J),RQL(J),TOD(1),HTS(1)
C
C *
C * *
C * * ADD THE CONTRIBUTIONS FROM THE CURRENT LINE TO THE CUMULATIVE RESULT.
C * *
  360 DO 370 I = 1,IMAX
      IF(I.LE.INUM)THEN
         RAW(I) = RAD(I)*H*C*VINIT
         SUM(I) = TRN(I)*H*C*VINIT
      END IF
      SUMPH(I) = SUMPH(I) + RAD(I)
  370 \text{ SUMRD(I)} = \text{SUMRD(I)} + \text{RAW(I)}
C * *
           *********
C *
```

```
C *
      IF ONLY ONE LINE IS CALCULATED, PRINT THE APPROXIMATE RESULT USED FOR
C *
      THE TAIL OF THE RADIANCE PROFILE.
C *
      IF(FLAG)THEN
          WRITE(4,125)(TRN(I), I=1, INUM)
          WRITE(4,123)(SUM(I),I=1,INUM)
          WRITE(4,100)
      END IF
C *
C *
      PRINT OUT THE RADIANCE---BOTH THE THIN-LINE APPROXIMATION AND THE RE-
С
      SULT OF THE FULL CALCULATION, WHENEVER IT IS PERFORMED. THE FORMER IS
C *
      USED ONLY WHEN THE LATTER IS BYPASSED.
C *
      IF(J.EQ.1.AND.LCNT.EQ.1)THEN
          WRITE(4,113)(HTS(I),HTS(I),I=1,IMAX)
          WRITE(4,121)(BL, I=1, IMAX)
          WRITE(4,101)
      END IF
      WRITE(4,111)BR(J),RQL(J),(THR(I),I=1,IMAX)
      IF(INUM.GT.0)WRITE(4,112)(RAW(I),I=1,INUM)
      IF(FLAG)THEN
          WRITE(4,100)
          DO 399 I = 1,3
          WRITE(4,129)(AST, K=1, IMAX)
  399
          GO TO 400
      END IF
C**
C**
      PRINT OUT THE TOTAL OPTICAL DEPTHS AT THE LINE CENTERS AND THE ACCUM-
C**
      ULATING RADIANCE (SUMRD) FOR EACH PATH. ALSO PRINT THE CPU TIME USED
C**
      AND THE INTEGRATION-PANEL INDICES. ALL THIS GOES TO UNIT 5.
C**
      IF(J.EQ.1.AND.LCNT.EQ.1)THEN
          WRITE(5,115)(HTS(I), I=1, IMAX)
          WRITE(5,114)(BL, I=1, IMAX)
          WRITE(5,101)
      END IF
      TS = SECOND() - TZ
      WRITE(5,116)TS,BR(J),RQL(J),LBND,(LMAX(I),KM(I),SUMRD(I),TOD(I),
     li=1,IMAX)
C**
C**
      IF SPECTRAL RADIANCE IS BEING CALCULATED, CALL SPEC1 TO ADD THE CON-
C**
      TRIBUTION FROM THE CURRENT LINE TO THE RESULTS PREVIOUSLY OBTAINED.
C**
      NNN = NR
      IF(FWHM.GT.0.0.AND.NNN.LE.3)CALL SPEC1(FWHM, VINIT, NNN, IMAX, RAW)
C**
  400 CONTINUE
C**
C**
      END THE LOOP (INDEX J) THAT CHOOSES DIFFERENT LINES
C**
C+ *******************************
C*
      IF MORE THAN 500 LINES ARE USED, BRANCH TO LINES3 TO REREAD THE NEXT
C*
      BATCH, AND THEN ENTER THE LOOP DO 400 ONCE AGAIN. LCNT IS THE NUMBER
C*
C*
      OF TIMES THIS LOOP IS ENTERED.
      IF(JMAX.LT.DIML)GO TO 490
      CALL LINES3(LCNT)
      LCNT = LCNT + 1
      IF(JMAX.EQ.0)GO TO 490
```

```
FLAG = .FALSE.
      GO TO 225
C*
      WRITE THE FINAL RESULTS FOR THE BAND RADIANCE FOR THE CURRENT GROUP
C*
ć*
      OF PATHS.
C*
  490 IF(FLAG)GO TO 500
      WRITE(4,100)
DO 491 I = 1,3
  491 WRITE(4,129)(AST,K=1,IMAX)
      WRITE(4,117)
      WRITE(4,119)(SUMRD(I),I=1,IMAX)
      WRITE(4,120)(SUMPH(I), I=1, IMAX)
      JMAX = JMAX + DIML*(LCNT-1)
      WRITE(4,118)JMAX,JCNT
C$
      IF (CMPL)
      DO 492 I = 1,3
  492 WRITE(9,129)(AST,K=1,IMAX)
      WRITT(9,117)
      WRITE(9,119)(SUMRD(1), I=1, IMAX)
      WRITE(9,120)(SUMPH(I), I=1, IMAX)
      WRITE(9,118) JMAX, JCNT
      DO 498 I = 1,3
  498 WRITE(9,129)(AST,K=1,IMAX)
      ENDIF
      DO 499 I = 1,3
  499 WRITE(4,129)(AST,K=1,IMAX)
С
      WRITE(4,100)
  500 CONTINUE
C*
C*
      END THE LOOP (INDEX NR) SELECTING DIFFERENT GROUPS OF VIEWING PATHS
C*
C *****
C
С
      IF SPECTRAL RADIANCE IS BEING CALCULATED, CALL SPEC2 TO WRITE IT TO
      UNITS 4 AND 7.
C
С
      IF(FWHM.GT.0.0)CALL SPEC2(FWHM)
C
      ***********
C
  998 IF(JMAX.EQ.0)THEN
          WRITE(4,990)
          WRITE(6,990)
      END IF
      CLOSE(1)
      CLOSE(2)
      CLOSE(3)
      REWIND(4)
      REWIND(5)
      REWIND(6)
      CLOSE(4)
      CLOSE(5)
      CLOSE(6)
      END
```

```
SUBROUTINE LINES(VIBE, VIBL, BRNCH)
C
C
000
       THE PURPOSE OF SUBROUTINE LINES IS TO PERFORM INITIALIZATION STEPS
                                                    READ UNIT 1
C
                                                    CALL ATMPR
                                                    READ UNIT 3
0000
                                                    CALL SPECTRM
                                                    SET COMMON/B/
C
       INTEGER RQL, DEGV, GL, GU, DIML
      LOGICAL CMPL, FLAG
      PARAMETER (DIML=500, CMPL=.FALSE.)
      CHARACTER*2 BR, BRNCH(DIML), BCH
      CHARACTER*3 MOL
       CHARACTER*4 UNIT
      CHARACTER*8 UST, LST, US, LS
      CHARACTER*10 MES(2), DATE, TIME
      CHARACTER*47 FMT, MSG
С
      DIMENSION V(DIML), STS(DIML), ALF(DIML), EDP(DIML), RQL(DIML), HGTS(50)
      COMMON/B/V,STS,ALF,EDP,RQL,NRL,HGTS,ACC,NPTS,NDP,
                WGT, LOOK, NREPS, IMXX, JMAX, FWHM
      SAVE UST, LST, ISO, BR, VMIN, VMAX, JNUM, FMT
   97 FORMAT(1H1, 'PROGRAM NLTE FOR INFRARED RADIANCE',
      1/, 'DATE = ', AlO, 'TIME = ', AlO, /)
   98 FORMAT(1H1)
   1'*******************,A2,/,' TAPE',I1)
  100 FORMAT(//, ' 1A---LINE DIRECTIVES: ',/,
     1/,' MOL = MOLECULE CODE =',3X,A3,
2/,' ISO = ISOTOPE CODE =',16,
3/,' UST = UPPER VIB LVL = ',A8,
     4/,' LST = LOWER VIB LVL = ',A8,
5/,' BR = RO-VIB BRANCH = ',4X,A2,
6/,' NRL = ROT''L LINE # = ',16)
  101 FORMAT(//, ' 1B---VIEWING PATH PARAMETERS: ',/,
     1/,' TANI = LOWEST ',A7,' HEIGHT (KM) =',F7.2,
2/,' TANF = HIGHEST ',A7,' HEIGHT (KM) =',F7.2,
      3/, 'SPAC = EXAMINATION INTERVAL (KM) = ', F7.2,
  4/,' LOOK =',I2,'; LOOKING GEOMETRY CHOSEN =',A7)
102 FORMAT(//,' 1C---PROGRAM PARAMETERS: ',/,
     FORMAT(//, ' 1C---PROGRAM PARAMETERS: ',/,
1/,' HMAX = ASSUMED TOP OF ATMOSPHERE (KM) =',15,5X,A16,
     2/, ACC = ACCURACY (INTEG''D RADIANCE) =', F7.5,
      3/, 'NPTS = NUMBER OF INTEG POINTS PER PANEL = ', 13,
      4/,' NDP =',12,'; LINESHAPE OPTION SELECTED =',A22,
     5/,' VMIN = LOWER END, LINE SEARCH (CM-1) =',16,6/,' VMAX = UPPER END, LINE SEARCH (CM-1) =',16)
  103 FORMAT(//, ' 1E---BAND PARAMETERS:
                                               ',A47,/,
     1/,' VIBE = VIB ENERGY OF THE TRANSITION (CM-1) =',Fl0.4,
      2/,' VIBL = VIB ENERGY OF THE LOWER STATE (CM-1) =',F10.4,
     3/,' VIBQ = QUANTUM FOR THE PARTITION FN (CM-1) =',Fl0.4,
      4/, GL = STATISTICAL WEIGHT, LOWER VIBRATIONAL STATE = ', 12,
               = STATISTICAL WEIGHT, UPPER VIBRATIONAL STATE = ',12)
  104 FORMAT(//, 'QUANTITIES RETURNED FROM MOLEC: ',/,
```

```
1',' WGT = MOLECULAR WEIGHT =', I4,
      2/, AI = ISOTOPIC ABUND = ',F7.5,
3/, DEGV (EXPLAINED IN MOLEC) = ',I4,
      4/,' PROT (EXPLAINED IN MOLEC) =',F4.1,
      5/, TEXP (EXPLAINED IN MOLEC) = ',F4.2)
  105 FORMAT(/,' FORMAT FOR THE SEARCH OF THE LINETAPE IS',/,1X,A47,/)
106 FORMAT(//,' $$$$$ CARD 1E NEEDED BUT NOT FOUND,',
      1' RESULTS UNPREDICTABLE $$$$$',//)
  107 FORMAT(//, 'AFGL LINE FILE FOR SELECTED TRANSITION:',
     13X,A3,I6,2X,2(1X,A8),/)
  108 FORMAT(2X, 'BR LINE
                                 FREQUENCY
      l'STRENGTH WIDTH LS ENERGY',/,
      216X,'(CM-1)',14X,'(CM-1)
                                        (CM-1)',/)
  109 FORMAT(2X,A2,I5,F14.4,E11.3,F7.3,F12.4)
  110 FORMAT(//,' PRINT THE HEADERS AND FIRST DATA CARD-IMAGES FOUND ',
      1'ON INPUT UNITS',/)
  111 FORMAT(//, ' 1D---SYNTHETIC SPECTRUM PARAMETERS: ',/,
1/,' FWHM = WIDTH OF TRIANGULAR SCANNING FN (',A4,') = ',F7.3,
2/,' DEL = SPACING OF PTS IN SYNTH SPECTRM (',A4,') = ',F7.3)
  112 FORMAT(//, ' 1D---SYNTHETIC SPECTRUM PARAMETERS: ',/
     1/,' FWHM = 0, SYNTHETIC SPECTRUM NOT GENERATED')
  113 FORMAT(//,' $$$$ NOTE: ONLY 50 L-O-S PATHS CAN BE RUN',/)
C
C
C
       INITIALIZATION--UNITS 1-6 ARE ASSOCIATED WITH LOCAL FILES TAPE1-TAPE6
C
       OPEN(1)
       OPEN(2)
       OPEN(3)
       OPEN(4)
       OPEN(5)
       OPEN(6)
       REWIND(2)
       REWIND(3)
       MES(1) = DATE()
       MES(2) = TIME()
       WRITE(4,97)MES(1),MES(2)
       WRITE(5,97)MES(1),MES(2)
       WRITE(6,97)MES(1),MES(2)
       BCH =
       I = 1
       WRITE(4,99)BCH, I
C$
       IF(CMPL)
       OPEN(9,FILE='OUTPUT')
       WRITE(9,97)MES(1),MES(2)
       WRITE(9,99)BCH, I
CS
       ENDIF
       I = 5
       WRITE(5,99)BCH, I
       T = 6
       WRITE(6,99)BCH, I
       WRITE(6,110)
С
С
       READ IN MODELLING DATA FROM CARDS---UNIT 1
C**** CARD 1A LINE DIRECTIVES CARD---LIST-DIRECTED READ
```

```
MOL = MOLECULE CODE (INPUT AS 'CO2', ETC. INCLUDING QUOTES)
             = ISOTOPE CODE (INTEGER)
         ISO
            = UPPER VIB STATE (AFGL LINE FILE NOTATION; INCLUDE QUOTES)
         UST
        LST = LOWER VIB STATE (AFGL LINE FILE NOTATION; INCLUDE QUOTES)
             = BRANCH (P, Q, OR R) (INPUT AS 'P', ETC.)
         NRL = ROTATIONAL LINE NUMBER (INTEGER)
C
     WHEN BR = 'A', THE P, Q, AND R BRANCHES ARE ALL EVALUATED (DEFAULT)
     WHEN NRL = 999 ALL LINES IN THE CHOSEN BRANCH ARE EVALUATED (DEFAULT)
С
     INDIVIDUAL LINES CAN BE SELECTED BY SETTING BR TO 'P', 'Q', OR 'R'
     AND SETTING NRL EQUAL TO THE DESIRED LINE NUMBER.
C**** CARD 1B VIEWING PATH PARAMETERS CARD---LIST-DIRECTED READ
         TANI = SMALLEST TANGENT HEIGHT OR OBSERVATION HEIGHT (KM)
C
        TANF = GREATEST TANGENT HEIGHT OR OBSERVATION HEIGHT (KM)
         SPAC = EXAMINATION INTERVAL (KM) (DEFAULT = +1 KM)
C
     IN LIMB-LOOKING GEOMETRY THE LINE-OF-SIGHT PATH IS PARAMETERIZED BY A
     TANGENT HEIGHT (LOOK = 0); IN ZENITH-LOOK GEOMETRY IT IS PARAMETER-
      IZED BY AN OBSERVATION HEIGHT (LOOK = 1). IF SPAC > 0, LIMB-LOOK GEO-
     METRY IS ASSUMED; IF SPAC < 0, ZENITH-LOOK IS ASSUMED. IN THE LATTER
     CASE, ABS(SPAC) IS USED FOR THE EXAMINATION INTERVAL.
C**** CARD 1C PROGRAM PARAMETERS CARD---LIST-DIRECTED READ
        HMAX = ALTITUDE, "TOP" OF USEFUL ATMOSPHERE (KM: DEFAULT = 1001)
С
        ACC = FRACTIONAL ERROR ALLOWABLE, INTEGRATED INTENSITY IN A LINE
С
                                             (DEFAULT = .01; MAXIMUM = .05)
        NPTS = NUMBER OF INTEGRATION PTS PER PANEL (NU-INTEG; DEFAULT = 4)
С
        NDP = LINESHAPE CODE: VOIGT (NDP = 0; DEFAULT) OR DOPP (NDP = 1)
         VMIN = LOWER END, FREQUENCY RANGE SEARCHED FOR RO-VIB LINES (CM-1)
        VMAX = UPPER END, FREQUENCY RANGE SEARCHED FOR RO-VIB LINES (CM-1)
C
C
     ANY VALUE OF HMAX FALLING BETWEEN TANF AND THE LARGEST ALTITUDE FOUND
     IN THE ATMOSPHERIC PROFILE IS ACCEPTABLE. IF HMAX IS NOT WITHIN THESE
C
     LIMITS, THE PROGRAM ADJUSTS IT AND PRINTS A MESSAGE.
     ACC DETERMINES WHETHER TO ACCEPT THE THIN-LINE APPROXIMATION FOR THE
C
      INTEGRATED RADIANCE OF THE INDIVIDUAL LINES, OR NOT. (IF ACCEPTED THE
     MAIN CALCULATION IS BYPASSED AND THE RESULT IS OBTAINED A GREAT DEAL
     MORE QUICKLY.) THE CRITERION FOR ACCEPTANCE IS BASED ON THE EMPIRICAL
     OBSERVATION THAT THE FRACTIONAL ERROR IS ABOUT TAU/3, WHERE TAU IS
     THE OPTICAL DEPTH AT LINE CENTER ALONG THE L-O-S PATH. (THIS HOLDS
     FOR TAU < .5.) ACC ALSO DETERMINES WHERE TO CUT OFF THE NUMERICAL IN-
      TEGRATION AND SUBSTITUTE THE ANALYTICAL EXPRESSION FOR THE CONTRIBU-
     TION IN THE TAIL OF THE RADINCE PROFILE, WHEN THE THICK-LINE CALCUL-
     ATION IS PERFORMED.
C
     POSSIBLE VALUES OF NPTS ARE 2, 4, AND 8. THE PROGRAM CHANGES UNACCEP-
     TABLE VALUES TO ONE OF THESE.
     VMIN AND VMAX LIMIT THE LINE-FILE SEARCH TO A CERTAIN RANGE OF LINE
     POSITIONS. DEFAULT IS TO SEARCH THE ENTIRE FILE.
```

C**** CARD 1D SYNTHETIC SPECTRUM CARD---LIST-DIRECTED READ

```
FWHM = FULL WIDTH HALF MAX OF TRIANG SCAN FN (CM-1 OR UM: DEF = 0)
        DEL = SPACING OF PTS IN SYNTH SPECTRUM (CM-1 OR UM: DEF = 1 CM-1)
        UNIT = 'CM-1' OR 'UM ': ENERGY OR WAVELENGTH UNITS (DEF = 'CM-1')
     WHEN FWHM > 0, SUBROUTINE SPECTRM IS CALLED TO GENERATE A SYNTHETIC
     SPECTRUM, USING A TRIANGULAR SCANNING FUNCTION. THE ALGORITHM ASSUMES
     THAT FWHM IS MUCH GREATER THAN THE BREADTH OF THE INDIVIDUAL RADIANCE
     PROFILES. ONLY 3 PLACES AFTER THE DECIMAL ARE RETAINED IN THE VALUES
     OF FWHM AND DEL.
C**** CARD 1E BAND PARAMETERS CARD---LIST DIRECTED READ
        VIBE = VIBRATIONAL ENERGY (CM-1) OF THE RADIATIVE TRANSITION
С
        VIBL = VIBRATIONAL ENERGY (CM-1) OF THE LOWER STATE
C
        VIBQ = VIBRATIONAL QUANTUM (CM-1) IN THE PARTITION FUNCTION
            = STATISTICAL WEIGHT OF THE LOWER VIBRATIONAL STATE
        GL
             = STATISTICAL WEIGHT OF THE UPPER VIBRATIONAL STATE
        Y
                                                                     Х
          IMPORTANT NOTE:
С
        Х
С
        X
          CARD 1E IS SUPERFLUOUS FOR CERTAIN TRANSITIONS OF CO2 AND NO
        X BECAUSE THE ENERGIES AND STATISTICAL WEIGHTS OF MANY VIBRA-
Ç
           TIONAL LEVELS ARE STORED IN BLOCK DATA MOLPAR. IF THE PRO-
С
        X GRAM LOCATES THE PROPER QUANTITIES, THIS CARD IS NOT READ;
        X OTHERWISE IT IS READ. IF THE USER IS UNCERTAIN ABOUT WHETHER
C
                                                                     Х
           THE TRANSITION WILL BE FOUND IT IS BETTER TO INCLUDE IT, BE-
                                                                     Х
           CAUSE 1E IS THE LAST CARD-IMAGE ON TAPEL AND NO SUBSEQUENT
        Х
          INFORMATION CAN BE MISREAD IF THIS CARD IS NOT NEEDED.
                                                                     X
                                                                     Х
        SET DEFAULT VALUES FOR SOME PARAMETERS READ IN ON CARDS 1A-1D
C
     BR = 'A'
     NRL = 999
     TANF = -1.0
     SPAC = 1.0
     HMAX = 1001
     ACC = .01
     NPTS = 4
     NDP = 0
     FWHM = 0.0
     VMIN = 0.0
     VMAX = 20000.
     DEL = 1.0
     UNIT = 'CM-1'
     CALL HEADER(1)
С
C****1A
C****
     READ(1,*)MOL, ISO, UST, LST, BR, NRL
     WRITE(4,100)MOL, ISO, UST, LST, BR, NRL
```

```
C****1B
C****
      READ(1, *) TANI, TANF, SPAC
       IF(TANF.LT.TANI)TANF = TANI
       IF(SPAC.GE.0.0)THEN
           LOOK = 0
           MSG(1:7)
                            LIMB'
           MSG(8:14) = 'TANGENT'
           IF(SPAC.EQ.0.0)SPAC = 1.0
      ELSE
           LOOK = 1
           MSG(1:7) = 'ZENITH'
MSG(8:14) = 'OBSERV.'
           SPAC = ABS(SPAC)
      END IF
      WRITE(4,101)MSG(8:14), TANI, MSG(8:14), TANF, SPAC, LOOK, MSG(1:7)
C
      SET PARAMETERS RELATED TO L-O-S PATHS---HGTS, IMXX, NREPS
C
      DO 170 I = 1.50
      EGTS(I) = TANI + (I-1)*SPAC
      IF(HGTS(I).GT.TANF)GO TO 175
  170 \text{ IMXX} = I
      WRITE(4,113)
      WRITE(6,113)
  175 NREPS = IMXX/5
      IF((5*NREPS).NE.IMXX)NREPS = NREPS + 1
С
C****1C
C****
      READ(1,*)HMAX,ACC,NPTS,NDP,VMIN,VMAX
      MSG(32:47) =
      I = HMAX
      IF(I.EQ.1001)MSG(32:47) = '(RESET IN ATMPR)'
      HMAX = I
      IF(ACC.GT..05)ACC = .05
      IF (NPTS.GT.4) THEN
          NPTS = 8
      ELSE IF(NPTS.LT.4)THEN
          NPTS = 2
      END IF
      MSG(1:22) = '
                     VOIGT
      IF(NDP.EQ.1)MSG(1:7) = 'DOPPLER'
      IF(NDP.LT.0)MSG(12:22) = '(USE VWERF)'
      IF(FWHM.LT.0.0)FWHM = 0.0
      JMAX = INT(VMIN)
      N = INT(VMAX)
      WRITE(4,102)I,MSG(32:47),ACC,NPTS,NDP,MSG(1:22),JMAX,N
C
C****1D
C****
      READ(1, *) FWHM, DEL, UNIT
      IF (FWHM.GT.0.0) THEN
          FWHM = INT(1000.*FWHM + 0.5)/1000.
          DEL = INT(1000.*DEL + 0.5)/1000.
          WRITE(4,111)UNIT, FWHM, UNIT, DEL
      ELSE
          WRITE(4,112)
      END IF
```

```
С
      CALL MOLEC TO ESTABLISH VALUES OF QUANTITIES AND PROGRAM PARAMETERS
C
С
      UNIQUELY ASSOCIATED WITH THE RADIATING MOLECULE, AND TO SEE IF IT IS
С
      NECESSARY TO READ CARD 1E.
C
     CALL MOLEC(MOL, ISO, UST, LST, I, DEGV, PROT, TEXP, VIBE, VIBL, VIBQ,
                GL, GU, AI, FMT, FLAG)
C
      WGT = FLOAT(I)/6.02486E+23
      MSG = '(FOUND IN MOLPAR)'
      IF (FLAG) THEN
C****1E
C****
          READ(1, *, END=190) VIBE, VIBL, VIBQ, GL, GU
          MSG = '(READ IN)'
      END IF
      GO TO 195
  190 MSG = '$$$$ NEITHER IN MOLPAR NOR READ IN $$$$$'
      WRITE(4,106)
      WRITE(6,106)
  195 WRITE(4,103)MSG, VIBE, VIBL, VIBQ, GL, GU
C
C
      PRINT SOME OF THE PARAMETERS RETURNED FROM MOLEC
C
      WRITE(4,104)I,AI,DEGV,PROT,TEXP
      WRITE(4,105)FMT
      WRITE(4,99)
      WRITE(4,98)
C
      I = 2
      WRITE(4,99)BCH, I
C$
      IF(CMPL)
      WRITE(9,109)
      WRITE(9,99)BCH, I
C$
      ENDIF
C
      С
C
      CALL SUBROUTINE ATMPR TO READ IN AND PREPARE THE ATMOSPHERIC PROFILE.
      SEE INPUT REQUIREMENTS IN THE COMMENTS IN ATMPR.
C
С
C
      CALL ATMPR(MOL, AI, VIBE, VIBL, VIBQ, GL, GU, DEGV, PROT, TEXP, TANI, TANF,
     1HMAX)
C
C
C
C
C
      CARD 3
              AFGL LINE FILE CARDS---UNIT 3
      THIS SECTION READS THE AFGL LINE FILE AND SELECTS LINES OF INTEREST
C
      BASED ON THE CRITERIA SPECIFIED IN OF THE VIRIABLES READ ON CARD 1A.
C
      MOST OF THE VARIABLES READ IN (VINIT, ST, AL, ED...) ARE STORED IN
C
C
      ARRAYS (V, STS, ALF, EDP...)
C
              VINIT (V) = FREQUENCY OF VIBRATIONAL TRANSITION (CM-1)
С
C
              ST (STS) = LINE INTENSITY
                                                (CM-1/MOLECULE-CM2)
```

```
AL (ALF) = LORENTZ HALF-WIDTH AT 296 K AND 1 ATMOS
                                                         (CM-1/ATMOS)
C
              ED (EDP) = ENERGY OF THE LOWER RO-VIB'L STATE (CM-1)
                       = UPPER AND LOWER STATE QUANTUM DESIGNATIONS
              BCH (BRNCH) = BRANCH (P, Q, OR R)
С
              N (RQL) = ROTATIONAL LINE NUMBER
C
              I = ISOTOPE CODE
С
C
C
С
      PRINT HEADERS
C
      I = 3
      WRITE(4,98)
      WRITE(4,99)BCH, I
C$
      IF (CMPL)
      WRITE(9,109)
      WRITE(9,99)BCH, I
C$
      ENDIF
      WRITE(4,109)
      CALL HEADER(I)
      WRITE(6,109)
      WRITE(4,107)MOL, ISO, UST, LST
      WRITE(4,108)
C
      SHIFT UST AND LET TO RIGHT-JUSTIFIED CHARACTER VARIABLES. SET FLAG.
C
      CALL SHFT(UST,US)
      CALL SHFT(LST,LS)
      FLAG = (MOL.EQ.'H2O').OR.(MOL.EQ.'O3 ').OR.(MOL.EQ.'CH4')
C
      JMAX COUNTS THE TOTAL NUMBER OF LINES TO BE USED
С
      JNUM COUNTS THE TOTAL NUMBER OF LINES READ, USING J
      HMAX = VMIN
      TEXP = VMAX
      JMAX = 0
      J = 0
C**** 3
C****
  200 READ(3,FMT,END=998)VINIT,ST,AL,ED,US,LS,BCH,N,I
     J = J + 1
C
     CHECK THE LINEFILE FOR THE CORRECT ISOTOPE AND BAND, AND POSSIBLY
С
С
     FOR THE CORRECT BRANCH AND LINE. IF THE DOPPLER LINESHAPE OPTION
      (NDP = 1) IS SELECTED, THE LORENTZ LINEWIDTHS ARE SET TO ZERO.
C
     READ THE WHOLE FILE ON THE FIRST CALL. IF THERE ARE MORE THAN DIML
     LINES, THE END OF THE FILE WILL BE REREAD FROM ENTRY LINES3 WHEN
C
С
      IT IS NEEDED. JMAX IS THE TOTAL NUMBER OF LINES SELECTED. J IS
С
     THE TOTAL READ.
      IF(VINIT.LT.VMIN)GO TO 200
      IF(VINIT.GT.VMAX)GO TO 200
      IF(ISO.NE.I) GO TO 200
      IF(UST.NE.US)GO TO 200
      IF(LST.NE.LS)GO TO 200
      IF(BR.NE.'A'.AND.BR.NE.BCH) GO TO 200
      IF(NRL.NE.N.AND.NRL.NE.999) GO TO 200
C
```

```
JMAX = JMAX + 1
      IF (FLAG) THEN
          BCH = '#
          N = JMAX
      END IF
      WRITE(4,109)BCH, N, VINIT, ST, AL, ED
      IF(VINIT.LT.TEXP)TEXP = VINIT
      IF(VINIT.GT.HMAX)HMAX = VINIT
      IF(JMAX.GT.DIML)GO TO 200
      JNUM = J
      V(JMAX) = VINIT
      STS(JMAX) = ST
      ALF(JMAX) = AL
      IF(NDP.EQ.1)ALF(JMAX) = 0.0
      EDP(JMAX) = ED
      BRNCH(JMAX) = BCH
      RQL(JMAX) = N
      GO TO 200
  998 VMIN = TEXP
      VMAX = HMAX
      WRITE(4,109)
      WRITE(4,99)
      CALL SPECTRM TO INITIALIZE FILES AND ARRAYS FOR THE SYNTHETIC SPEC-
C
С
      TRUM, IF NECESSARY. THEN RETURN TO NLTE.
      IF(JMAX.LE.1)FWHM = 0.0
      IF(FWHM.GT.0.0)CALL SPECTRM(VMIN, VMAX, DEL, FWHM, UNIT,
                                   MOL, ISO, UST, LST, BR, HGTS, IMXX, LOOK, MES)
      RETURN
С
С
С
C
      ENTRY TO REREAD THE PART OF THE LINEFILE PAST THE FIRST DIML LINES
C
      ENTRY LINES3(LCNT)
С
      SKIP PAST THE HEADER AND THE LINES ALREADY READ
С
С
      CALL REWND(3)
      DO 295 J = 1,JNUM
  295 READ(3,109)BCH
C
      REREAD THE NEXT BATCH OF LINES
С
C
      JMAX = 0
  300 READ(3,FMT,END=999)VINIT,ST,AL,ED,US,LS,BCH,N,I
      JNUM = JNUM + 1
      IF(VINIT.LT.VMIN)GO TO 300
      IF(VINIT.GT.VMAX)GO TO 300
      IF(ISO.NE.I) GO TO 300
      IF(UST.NE.US)GO TO 300
      IF(LST.NE.LS)GO TO 300
      IF(BR.NE.'A'.AND.BR.NE.BCH) GO TO 300
      IF(NRL.NE.N.AND.NRL.NE.999) GO TO 300
С
      JMAX = JMAX + 1
      V(JMAX) = VINIT
```

```
STS(JMAX) = ST
ALF(JMAX) = AL
IF(NDP.EQ.1)ALF(JMAX) = 0.0
EDP(JMAX) = ED
BRNCH(JMAX) = BCH
RQL(JMAX) = N
IF(FLAG)THEN
BRNCH(JMAX) = '#'
RQL(JMAX) = JMAX + DIML*LCNT
END IF
IF(JMAX.LT.DIML)GO TO 300
999 RETURN

C
END
END
```

lTANF, HMAX) С C SUBROUTINE FOR READING, ORGANIZING, AND PRINTING THE ATMOSPHERIC PRO-C FILE FOUND ON TAPE2, AND FOR SETTING UP COMMON/A/. OF THE TOTAL CON-TENTS OF /A/, ONLY THE FIRST 7 (OUT OF 13) ARRAYS, PLUS THE ORDINARY С VARIABLES ARE NEEDED BY THE MAIN PROGRAM. C2 AND BST ARE SET IN THE C MAIN PROGRAM. C ******** Ċ THE DATA WHICH MAY BE READ ARE: C С * ALT ALTITUDE (KM) C * TRTMP TRANSLATIONAL TEMPERATURE (KELVIN) * RHO TOTAL NUMBER DENSITY OF RADIATING MOLECULE (CM-3) NUMBER DENSITY OF LOWER VIBRATIONAL LEVEL (CM-3) (REAL) NUMBER DENSITY OF UPPER VIBRATIONAL LEVEL (CM-3) (REAL) С NT. C C NU **TVL VIBRATIONAL TEMPERATURE DESCRIBING LOWER LEVEL (KELVIN) С * TVU VIBRATIONAL TEMPERATURE DESCRIBING UPPER LEVEL (KELVIN) C * TVQ VIBRATIONAL TEMPERATURE DESCRIBING LOWEST EXCITED LEVEL (K) С NO NUMB DENS, GROUND VIBRATIONAL LEVEL (CM-3) (FOR P FN; REAL) NUMB DENS, FIRST EXCITED VIB LEVEL (CM-3) (FOR P FN; REAL) C C THESE QUANTITIES ARE NOT ALL REQUIRED. THE ATMOSPHERIC PROFILES MAY BE DEFINED IN TERMS OF NUMBER DENSITIES OR VIBRATIONAL TEMPERATURES, C AND THE PROGRAM AUTOMATICALLY RECOGNIZES CERTAIN COMBINATIONS WHICH ARE LISTED BELOW. (SEE THE LATER COMMENTS.) THE QUANTITIES WITH SIN-GLE ASTERISKS ARE DIRECTLY USED BY NLTE (FOR HOT BANDS, TVL IS ALSO). THEY MUST THEREFORE BE READ DIRECTLY OR CALCULATED BY ATMPR. FOR REGULAR BANDS, POSSIBLE PROPER COMBINATIONS OF INPUT DATA ARE: C NVP NPF C INDEX 1. ALT, TRTMP, RHO, TVU, TVQ 1 1 2. ALT,TRTMP,RHO,TVU,NO,N1
3. ALT,TRTMP,NL,NU,TVQ
4. ALT,TRTMP,NL,NU,NO,N1 2 С 7 C 1 C 2 C IN ADDITION, FOR REGULAR BANDS THE PROGRAM WILL ACCEPT: C 5. ALT, TRTMP, RHO, TVU 6. ALT, TRTMP, NL, NU C FOR HOT BANDS, POSSIBLE COMBINATIONS ARE: 7. ALT, TRTMP, RHO, TVL, TVU, TVQ 1 8. ALT, TRTMP, RHO, TVL, TVU, NO, N1
9. ALT, TRTMP, RHO, NL, NU, TVQ С 2 10. ALT, TRTMP, RHO, NL, NU, NO, N1 2 FOR EITHER REGULAR OR HOT BANDS, LTE CONDITIONS ARE IMPLIED BY 11. ALT, TRTMP, RHO 3

SUBROUTINE ATMPR(MOL, AI, VIBE, VIBL, VIBO, GL, GU, DEGV, PROT, TEXP, TANI,

С C C С C С С С C C C C C C C С C C C C C С С С С C С C č C C

C

С

THE FORMAT FOR ALL THESE POSSIBILITIES IS (F5.1,F10.3,5E12.5). THE PROGRAM IDENTIFIES THE OPTION SELECTED AND CALCULATES THE REQUIRED QUANTITIES WHICH ARE NOT DIRECTLY READ IN. IN THE CASE OF OPTIONS 5 AND 6, APPROXIMATIONS ARE NECESSARILY MADE UNLESS THE RADIATING LEVELS ARE THE GROUND AND FIRST EXCITED VIBRATIONAL STATES. THAT IS, THE VIBRATIONAL PARTITION FUNCTION WILL BE CALCULATED USING THE TWO RADIATING STATES INSTEAD OF THE GROUND AND FIRST EXCITED STATES, AND IT WILL BE SLIGHTLY IN ERROR AS A RESULT. SEE THE COMMENTS IN THE OUTPUT.

FOR HOT BANDS IN WHICH THE VIBRATIONAL TEMPERATURES, TVL AND TVU, CAN BE ASSUMED IDENTICAL, ZEROES IN THE TVU DATA FIELD WILL RESULT IN DATA FOR TVL BEING USED FOR TVU AS WELL (OPTIONS 7 AND 8 ONLY).

## IMPORTANT NOTE:

THE NUMBER DENSITIES NL AND NU REFLECT THE ABUNDANCE OF THE ISOTOPE UNDER CONSIDERATION. RHO, ON THE OTHER HAND, IS THE TOTAL NUMBER DENSITY OF THE SPECIE, INCLUDING ALL ISOTOPES.

## ANOTHER IMPORTANT NOTE:

THE PROGRAM AUTOMATICALLY DISTINGUISHES AMONG THE ELEVEN CASES CITED ABOVE. IT DOES SO BY READING THE FIRST DATA CARD-IMAGE (CORRESPONDING TO THE LOWEST ALTITUDE ON THE ATMOSPHERIC-PROFILE DATA FILE) AND LOOKING AT NUMERICAL VALUES OF SOME OF THE QUANTITIES READ. THE CRITERIA USED TO DISTINGUISH BETWEEN THE VARIOUS CASES ARE GIVEN BELOW, FOLLOWED BY THE RULES FOR INTERPRETING THE FIELDS AND FIXING THE CORRESPONDING VALUES OF NVP AND NPF. THE INTERPRETATIONS ARE MADE IN SUBROUTINE OPTION AND PRINTED AS DIAGNOSTIC OUTPUT ON UNIT 6.

THE NUMERICAL VALUE, X, FOUND IN THE 5TH DATA FIELD (6TH, FOR HOT BANDS) IS USED TO DETERMINE NPF:

- (A) IF X.LE.O, DATA FOR THE PARTITION FUNCTION ARE ABSENT, SET NPF = 0.
- (B) IF 0<X<10000, FIELD 5 (6 FOR HOT BANDS) IS ASSUMED TO BE A VI-BRATIONAL TEMPERATURE, TVQ. SET NPF = 1.
- (C) IF X.GE.10000, FIELDS 5 AND 6 (6 AND 7 FOR HOT BANDS) ARE ASSUMED TO BE NUMBER DENSITIES, NO AND N1.

  SET NPF = 2.

THE NUMERICAL VALUE, Y, FOUND IN THE 4TH DATA FIELD IS USED TO DETERMINE NVP:

- (D) IF Y.LE.O, DATA FOR THE RADIATING LEVELS ARE ABSENT, AND LTE CONDITIONS ARE ASSUMED (ALSO FOR THE PARTITION FUNCTION, REGARDLESS OF CRITERIA (A)-(C).) COLUMN 3 IS INTERPRETED AS THE TOTAL NUMBER DENSITY, RHO. SET NVP = 3.
- (E) IF 0<Y<1000, FIELD 4 IS ASSUMED TO BE A VIBRATIONAL TEMPERA-TURE, TVU (FIELDS 4 AND 5 FOR HOT BANDS, TVL AND TVU). FIELD 3 IS THE TOTAL NUMBER DENSITY, RHO, IN EITHER CASE, SET NVP = 1.
- (F) IF Y.GE.1000, FIELDS 3 AND 4 (4 AND 5 FOR HOT BANDS) ARE AS-SUMED TO BE NUMBER DENSITIES, NL AND NU.

```
SET NVP = 2.
С
      OVERRIDES:
С
                  IT IS POSSIBLE TO OVERRIDE ANY OF THE RULES LISTED ABOVE
      WITH THE CRITERIA (A) THRU (F) BY ENTERING CERTAIN CHARACTER DATA
      ANYWHERE WITHIN A FIELD COMPRISING COLUMNS
                                                       76 THROUGH 90 (ON THE
      LOWEST-ALTITUDE CARD ONLY). THERE ARE TWO COMMON REASONS FOR DOING
C
      THIS. FIRST, ONE MAY WISH TO CALCULATE RESULTS FOR LTE CONDITIONS
      REGARDLESS OF THE VIBRATIONAL TEMPERATURES OR NUMBER DENSITIES ON
      THE FILE. SECOND, FOR HIGH-LYING STATES THE NUMBER DENSITIES MAY
      ACTUALLY HAVE VALUES BELOW 1000 SO THAT CRITERIA (E) AND (F) COULD
C
      BE CONFUSED.
C
      ACCEPTABLE VALUES FOR THE OVERRIDE CHARACTER DATA ARE:
С
         SYMBOL
                    MEANING
С
С
                 LTE CONDITIONS PREVAIL
          LTE
C
                 RULES (B) AND (E) APPLY, REGARDLESS OF VALUES OF X AND Y
          T,T
С
                 RULES (B) AND (F) APPLY, REGARDLESS OF VALUES OF X AND Y
          T,N
                 RULES (C) AND (E) APPLY, REGARDLESS OF VALUES OF X AND Y
C
          N,T
                 RULES (C) AND (F) APPLY, REGARDLESS OF VALUES OF X AND Y
          N,N
С
C
      INTEGER A,GL,GU,DEGV
      REAL NO, N1, NL, NU
      CHARACTER*1 AST(5)
      CHARACTER*3 MOL
      CHARACTER*15 CODE
      DIMENSION DUM(250), TRTMP(250), PRESS(250), RHO(250), TVL(250)
      DIMENSION TVU(250), QV(250), NL(250), NU(250), TVQ(250), NO(250)
      DIMENSION N1(250), ALT(250), PR(192)
C
      COMMON/A/ALT, TRTMP, PRESS, RHO, TVL, TVU, QV, NL, NU, TVQ, NO, N1, DUM,
                KMAX,C2,BST,TMIN
      COMMON/P/PR
С
       ****
  100 FORMAT(BZ,F5.0,F10.3,5E12.5,A15)
  101 FORMAT(//,' $$$$$ ATMOSPHERIC PROFILE STARTS ABOVE TANI, ADJUST',
     1' TANI TO', F7.2, 'KM $$$$$',//)
  102 FORMAT(//, $$$$$ HMAX GREATER THAN ALTITUDE OF UPPERMOST '
     1'POINT OF ATMOSPHERIC PROFILE, RESET HMAX TO', F7.2, 'KM $$$$$',
  103 FORMAT(/,' INPUT OPTION #',13,'; NVP =',12,', NPF =',12,
1', VIBL ',A1,' 0; (SEE COMMENTS IN ATMPR)',/)
  104 FORMAT(//, 2X, ' $$$$$ SUBSTITUTE TVU FOR TVQ,
                                                         THE VIBRATIONAL '.
     1'TEMPERATURE USED IN FINDING THE PARTITION FUNCTION')
  105 FORMAT(9X, 'SMALL ERRORS WILL OCCUR IN ALL ABSORPTION CALCULAT',
  l'IONS (ALSO STARRED QUANTITIES IN PROFILE) $$$$$',//)
106 FORMAT(9X,'SMALL ERRORS WILL OCCUR IN PRINTED OUTPUT (STARRED',
     1' IN PROFILE) BUT NOT IN RADIANCE CALCULATIONS $$$$$',//)
7 FORMAT(10X,'ALT',5X,'TR TEMP VB TEMP',7X,'TOT PRESS',3X,A3,2X,
1'DENSITY LOWER STATE UPPER STATE 7B TEMP PART',/,
  107 FORMAT(10X, 'ALT', 5X, 'TR TEMP
     29X,'(KM)',2(7X,'(K)'),10X,'(ATMOS)',7X,'(CM-3)',2X,
32(8X,'(CM-3)'),10X,'(1)',7X,'FN')
  108 FORMAT(I4,F9.2,2X,2F10.3,2X,1P,2E14.4,2X,2E14.4,0P,F13.3,F9.5)
```

```
109 FORMAT(14,F9.2,2X,3F10.3,2X,1P,2E14.4,2X,2E14.4,0P,F13.3,F9.5)
  110 FORMAT(10X,'ALT',5X,'TR TEMP',5X,'TVL',7X,'TVU',9X,'TOT PRESS',
                                                           VB TEMP
     13X,A3,2X, 'DENSITY
                             LOWER STATE UPPER STATE
     2'PART',/,9X,'(KM)',3(7X,'(K)'),10X,'(ATMOS)',7X,'(CM-3)',3X,32(8X,'(CM-3)'),9X,'(1)',7X,'FN')
  111 FORMAT(53X,A1,17X,A1,13X,A1,12X,A1,9X,A1)
  112 FORMAT(63X,A1,17X,A1,13X,A1,12X,A1,9X,A1)
  113 FORMAT(//,' $$$$$ HMAX INCOMPATIBLE WITH TANF, ADJUST HMAX TO',
     1F5.0,' KM $$$$$',//)
  114 FORMAT(' THE LOWER- AND UPPER-STATE POPULATIONS REFLECT AN ',
     l'ABUNDANCE OF', F7.5, 'W.R.T. TOTAL', A3,/)
  115 FORMAT(//,' $$$$$ CAUTION---FOR HOT BANDS THE PARTITION FUNCTION',
     1' PARAMETERS MUST BE READ IN $$$$$',//)
  116 FORMAT(//,' $$$$$ CAUTION---ATMOSPHERIC PROFILE CONTAINS MORE',
     1' THAN 250 ENTRIES, UPPER REGIONS NOT READ $$$$$',//)
C
С
      WRITE(4,111)
C
      READ AND WRITE THE HEADER FROM TAPE2. THEN READ THE FIRST CARD-IMAGE (FORMAT(F5.1,F10.3,5E12.5,A15)). CALL SUBROUTINE OPTION TO INTERPRET
C
C
      THE QUANTITIES FOUND THERE. THE INTERPRETATION IS WRITTEN TO UNIT 6.
C
C**** 2A
C****
      CALL HEADER(2)
C
C**** 2B
2****
      READ(2,100)(DUM(1),I=1,7),CODE
      CALL OPTION(DUM, CODE, VIBL, NVP, NPF, INDEX)
      CALL REWND(2)
      ***********
C
      AST(1) = '='
      IF(VIBL.GT.0.0)AST(1) = '>'
      WRITE(4,103)INDEX,NVP,NPF,AST(1)
      WRITE(4,114)AI,MOL
      DO 175 I = 1,5
  175 AST(I) = '
      IX = 0
      E = AINT(TANI)
      IF(VIBL.GT.0.0)THEN
          IF(DUM(5).EQ.0.0.AND.NVP.EQ.1)IX = 99
          IF(DUM(6).EQ.0.0)THEN
              WRITE(4,115)
              WRITE(6,115)
          END IF
      END IF
C
C
C
      READ THE ATMOSPHERIC DATA---FORMAT(F5.1,F10.3,5E12.5)
C
C**** 2B
C****
  180 K = 1
      IF(VIBL.GT.0.0)GO TO 190
```

```
185 IF(K.GE.251)GO TO 199
      READ(2,100,END=200)ALT(K),TRTMP(K),RHO(K),TVU(K),NO(K),
     1N1(K)
      TVL(K) = 1.0E+90
      IF(ALT(K).GE.E)K = K + 1
      GO TO 185
  190 IF(K.GE.251)GO TO 199
      READ(2,100,END=200)ALT(K),TRTMP(K),RHO(K),TVL(K),TVU(K),
     1NO(K), N1(K)
      IF(ALT(K).GE.E)K = K + 1
      GO TO 190
      **************************
С
С
C
      CHECK TO SEE IF TANI FALLS ABOVE ALT(1). IF SO, CONTINUE. IF NOT,
      CHECK TO SEE IF THE LOWER BOUNDARY OF THE USEFUL ATMOSPHERE WAS
С
С
      CORRECTLY DETERMINED. (FOR ALTITUDE SPACINGS OF GREATER THAN 1 KM,
      IT MIGHT NOT BE.) IF CORRECTLY DETERMINED, RESET TANI. IF NOT, RE-
      WIND AND REREAD TAPE2 TO GET THE CORRECT PROFILE RANGE. ALSO, FIX
      THE INDEX, KMAX, CORRESPONDING TO THE ALTITUDE USED FOR THE "TOP" OF THE ATMOSPHERE, ADJUSTING THE "TOP" DOWNWARD IF THE PROFILE
      READ IN DOES NOT EXTEND AS FAR AS ANTICIPATED.
  199 WRITE(4,116)
      WRITE(6,116)
  200 \text{ KMAX} = K - 1
      IF(ALT(1).LE.TANI)GO TO 205
      IF(DUM(1).LE.TANI)THEN
          CALL REWND(2)
          DUM(1) = ALT(1)
          E = AINT(TANI - (ALT(2)-ALT(1)) + 1)
          GO TO 180
      ELSE
          TANI = ALT(1)
          WRITE(4,101)TANI
          WRITE(6,101)TANI
      END IF
  205 IF(HMAX.GE.TANF)GO TO 210
      HMAX = AINT(TANF+50)
      WRITE(4,113)HMAX
      WRITE(6,113)HMAX
  210 IF(HMAX.GT.ALT(KMAX))THEN
                                        RESET HMAX
С
          I = HMAX
          HMAX = ALT(KMAX)
          IF(I.NE.1001)THEN
              WRITE(4,102)HMAX
              WRITE(6,102)HMAX
          END IF
                                   'TANF TOO HIGH'
          IF(TANF.GE.HMAX)STOP
      ELSE IF(HMAX.LT.ALT(KMAX))THEN
C
                                        RESET KMAX
          I = KMAX
          DO 215 A = KMAX, 1, -1
          IF(ALT(A).LT.HMAX)GO TO 220
  215
          I = A
  220
          KMAX = I
      END IF
Ç
```

```
C
      DETERMINE THE PRESSURE, IN ATMOSPHERES, AT EACH ALTITUDE
      DO 280 A = 1,KMAX
      IP = INT(ALT(A))
      E = IP
      IF(IP.GT.300)THEN
          PRESS(A) = 0.0
      ELSE IF(IP.GT.191)THEN
          PRESS(A) = PR(192) * EXP((191.-ALT(A))/4.4)
      ELSE IF(E.EQ.ALT(A))THEN
          PRESS(A) = PR(IP+1)
      ELSE
          E = ALOG(PR(IP+1))
          QVIB = ALOG(PR(IP+2))
          Z1 = IP
          22 = 21 + 1.0
          CALL LINT(ALT(A),F,E,QVIB,Z1,Z2)
          PRESS(A) = EXP(F)
      END IF
  280 CONTINUE
С
C
      FIND THE VIBRATIONAL TEMPERATURE FOR THE PARTITION FUNCTION, TVO
C
      IF(NPF.EQ.3)THEN
          DO 305 A = 1,KMAX
          TVQ(A) = TRTMP(A)
  305
      ELSE IF(NPF.EQ.2)THEN
          CALL VIBTMP(C2,1,KMAX,VIBQ,DEGV,N0,N1,TVQ)
      ELSE IF(NPF.EQ.1)THEN
          DO 310 A = 1, KMAX
          TVQ(A) = NO(A)
  310
      ELSE IF (INDEX.EQ.6) THEN
          CALL VIBTMP(C2,1,KMAX,VIBE,GU,RHO,TVU,TVQ)
          IF(VIBE.NE.VIBQ)THEN
              WRITE(4,104)
              WRITE(4,106)
              WRITE(6,104)
              WRITE(6,106)
              WRITE(4,108)
              AST(1) = AST(4) = AST(5) = '*'
          END IF
      ELSE
          DO 315 A = 1,KMAX
  315
          TVQ(A) = TVU(A)
          IF(VIBE.NE.VIBQ)THEN
              WRITE(4,104)
              WRITE(4,105)
              WRITE(6,104)
              WRITE(6,105)
              WRITE(4,108)
              AST(2) = AST(3) = AST(4) = AST(5) = '*'
          END IF
      END IF
C
Ç
      CALCULATE THE VIBRATIONAL PARTITION FUNCTION
      DO 320 A = 1,KMAX
```

```
320 QV(A) = 1.0/(1.0 - EXP(-C2*VIBQ/TVQ(A)))**DEGY
C
C
C
C
      CALCULATE AND PRINT THE ATMOSPHERIC PROFILE FOR REGULAR BANDS
С
      IF(VIBL.GT.0.0)GO TO 400
      WRITE(4,107)MOL
      WRITE(4,111)(AST(I), I=1,5)
С
      IF(NVP.EQ.4)THEN
          DO 340 A = 1,KMAX
          TVU(A) = TRTMP(A)
  340
          RHO(A) = RHO(A)*QV(A)/AI
      ELSE IF(NVP.EQ.3)THEN
          DO 345 A = 1, KMAX
          TVU(A) = TRTMP(A)
  345
      ELSE IF(NVP.EQ.2)THEN
          DO 350 A = 1,KMAX
          NL(A) = RHO(A)
          NU(A) = TVU(A)
  350
          RHO(A) = RHO(A)*QV(A)/AI
      END IF
С
      IF(NVP.EO.2)THEN
          CALL VIBTMP(C2,1,KMAX,VIBE,GU,NL,NU,TVU)
          CALL VIBPOP(C2,1,KMAX,AI,VIBL,GL,RHO,QV,TVL,NL)
          CALL VIBPOP(C2,1,KMAX,AI,VIBE,GU,RHO,QV,TVU,NU)
      END IF
С
      DO 360 A = 1,KMAX
  360 WRITE(4,108)A,ALT(A),TRTMP(A),TVU(A),PRESS(A),RHO(A),NL(A),NU(A),
     lTVQ(A),QV(A)
      GO TO 490
С
С
С
С
      CALCULATE AND PRINT THE ATMOSPHERIC PROFILE FOR HOT BANDS
C
  400 WRITE(4,110)MOL
      WRITE(4,112)(AST(I),I=1,5)
С
      IF(NVP.EQ.3)THEN
          DO 445 A = 1, KMAX
          TVL(A) = TRTMP(A)
          TVU(A) = TRTMP(A)
  445
      ELSE IF(NVP.EQ.2)THEN
          DO 450 A = 1,KMAX
          NL(A) = TVL(A)
          NU(A) = TVU(A)
  450
          DUM(A) = AI*RHO(A)/QV(A)
С
      ELSE IF(IX.EQ.99)THEN
          DO 455 A = 1,KMAX
          TVU(A) = TVL(A)
  455
      END IF
С
      E = VIBL + VIBE
      IF(NVF, EQ. 1.OR. NVF, EQ. 3) THEN
```

```
CALL VIBPOP(C2,1,KMAX,AI,VIBL,GL,RHO,QV,TVL,NL)
          CALL VIBPOP(C2,1,KMAX,AI,E,GU,RHO,QV,TVU,NU)
      ELSE
          CALL VIBTMP(C2,1,KMAX,VIBL,GL,DUM,NL,TVL)
          CALL VIBTMP(C2,1,KMAX,E,GU,DUM,NU,TVU)
      END IF
C
      DO 460 A = 1.KMAX
  460 WRITE(4,109)A,ALT(A),TRTMP(A),TVL(A),TVU(A),PRESS(A),RHO(A),NL(A),
     lNU(A),TVQ(A),QV(A)
C
  490 CONTINUE
C
С
      THE ARRAYS RHO AND PRESS ARE CONVERTED TO THE GEOMETRIC MEAN DENSITY
      IN THE LAYER WHOSE BOUNDARIES ARE A AND A+1, AND STORED WITH INDEX A.
      THE ARRAYS TRTMP, TVL, AND TVU ARE CONVERTED TO AVERAGE TEMPERATURES
C
      IN THE LAYER WHOSE BOUNDARIES ARE A AND A + 1. THESE AVERAGE TEMPERA-
C
      TURES ARE ALSO MULTIPLIED BY
                                    1/C2 (SEE COMMENT IN THE MAIN PROGRAM:
      THIS FACTOR APPEARS WHENEVER THE TEMPERATURES ARE USED) AND ARE STOR-
C
C
      ED IN THE SAME ARRAYS. AS WITH RHO AND PRESS, THE INDEX FOR THE LAYER
      WHOSE BOUNDARIES ARE ALT(A) AND ALT(A+1) KM ABOVE THE EARTH'S SURFACE
С
C
C
      OV BECOMES AN ARRAY STORING THE PRODUCT OF TWO RATIOS:
                    THE VIBRATIONAL PARTITION FUNCTION AT TS
                                                               (QVIB) TO
C
                    THE VIBRATIONAL PARTITION FUNCTION AT TVQ (QV(A))
č
      AND
                    THE ROTATIONAL PARTITION FUNCTION AT TS TO
                    THE ROTATIONAL PARTITION FUNCTION AT TRTMP
С
C
      THE LATTER RATIO IS A POWER OF THE RATIO OF TEMPERATURES.
                                                                  TS/TRTMP.
      WHERE TRIMP IS THE ACTUAL TRANSLATIONAL TEMPERATURE (NOT MULTIPLIED
C
С
      BY 1/C2) AND TS = 296 K. THE EXPONENT IS PROT.
      PRESS(A) IS INITIALLY THE TOTAL PRESSURE, IN ATMOSPHERES. AT STATE-
      MENT 500, IT BECOMES AN ARRAY STORING THE FACTOR BY WHICH THE LORENTZ
      LINEWIDTH PARAMETER (GIVEN ON THE LINE FILE AT TS AND 1 ATMOSPHERE)
      IS MULTIPLIED TO CORRECT FOR PRESSURE AND TEMPERATURE AT VARIOUS AL-
      TITUDES.
      QVIB = 1.0/(1.0 - EXP(-VIBQ/BST))**DEGV
      KMAX = KMAX - 1
      E = 1.0 - TEXP
      TMIN = 1.0E+10
      DO 500 A = 1,KMAX
      RHO(A)
             = SQRT(RHO(A)*RHO(A+1))
      PRESS(A) = SQRT(PRESS(A)*PRESS(A+1))
      TRTMP(A) = 0.5*(TRTMP(A) + TRTMP(A+1))/C2
      IF(TRTMP(A).LT.TMIN)TMIN = TRTMP(A)
      TVL(A) = 0.5*(TVL(A) + TVL(A+1))/C2
      TVU(A) = 0.5*(TVU(A) + TVU(A+1))/C2
      TVQ(A) = 0.5*(TVQ(A) + TVQ(A+1))/C2
     QV(A) = 1.0/(1.0 - EXP(-VIBQ/TVQ(A)))**DEGV
      QV(A) = (QVIB/QV(A))*(BST/TRTMP(A))**PROT
  500 PRESS(A) = PRESS(A)*(BST/TRTMP(A))**E
     TMIN = ANINT(TMIN*C2)
C
     RETURN
     END
```

```
SUBROUTINE OPTION(DUM, CODE, VIBL, NVP, NPF, INDEX)
         SUBROUTINE OPTION DETERMINES THE INPUT OPTIONS FOR THE ATMOSPHERIC
         PROFILE. IT READS THE FIRST DATA CARD-IMAGE---THAT IS, THE CARD-IMAGE
        CONTAINING THE ATMOSPHERIC PROPERTIES AT THE LOWEST ALTITUDE ON THE FILE--AND DECIDES, ON THE BASIS OF THE NUMERCAL VALUES READ AND THE TYPE OF BAND UNDER CONSIDERATION, WHAT THE UNDETERMINED QUANTITIES MUST BE. THEN THE OVERRIDE CODE IS CHECKED TO SEE IF THESE DEFAULT
         INTERPRETATIONS NEED TO BE CHANGED.
         CHARACTER*1 B1,B2
         CHARACTER*3 COD
         CHARACTER*12 MSG(9),MSH(5)
         CHARACTER*15 CODE
         DIMENSION DUM(250)
                                      TOT # DENS',' LST V TEMP',' UST V TEMP',
LST # DENS',' UST # DENS',' 1ST V TEMP',
GST # DENS',' 1ST # DENS',' NOT USED '/
        DATA (MSG(I), I=1,9)/'
   100 FORMAT(1X, 'ALT
                                  TR TEMP', 5A12, A15, 33X, '(INTERP)')
        DISSECT THE OVERRIDE CODE
        CALL SHFT(CODE, CODE)
        B1 = CODE(15:15)
IF(B1.EQ.''')THEN
              CODE(15:15) = ' '
              CALL SHFT(CODE, CODE)
        END IF
        COD = CODE(13:15)
        B1 = CODE(13:13)
B2 = CODE(15:15)
        CHECK THE FIRST ATMOSPHERIC DATA RECORD TO ESTABLISH THE INPUT OPTION
        USED. IGNORE OVERRIDES FOR NOW.
        E = DUM(5)
        IF(VIBL.GT.0.0)E = DUM(6)
C
        IF(E.LE.O.O)THEN
             NPF = 0
        ELSE IF(E.LT.10000.) THEN
             NPF = 1
        ELSE
             NPF = 2
        END IF
        E = DUM(4)
        IF(E.LE.O.O)THEN
             NVP = 3
             NPF = 3
        ELSE IF(E.LT.1000.) THEN
            NVP = 1
        ELSE
             NVP = 2
        END IF
С
        INITIALIZE MESSAGE ARRAYS
```

```
IF(COD.EQ.'LTE')THEN
          MSG(2) = MSG(3) = MSG(5) = MSG(6) = MSG(7) = MSG(8) = MSG(9)
      END IF
      DO 190 I = 1,5
  190 \text{ MSH}(I) = '
C
С
      SET THE INTERPRETIVE MESSAGES FOR REGULAR BANDS
С
      IF(VIBL.EQ.0.0)THEN
С
          IF(NVP.EQ.1)THEN
              MSH(1) = MSG(1)
              MSH(2) = MSG(3)
          ELSE IF(NVP.EQ.2)THEN
              MSH(1) = MSG(4)
              MSH(2) = MSG(5)
          ELSE
              MSH(1) = MSG(1)
          END IF
С
          IF(NPF.EQ.1)THEN
              MSH(3) = MSG(6)
          ELSE IF(NPF.EQ.2)THEN
              MSH(3) = MSG(7)
              MSH(4) = MSG(8)
          END IF
C
С
      SET THE INTERPRETIVE MESSAGES FOR HOT BANDS
      ELSE
          MSH(1) = MSG(1)
          IF(NVP.EQ.1)THEN
              MSH(2) = MSG(2)
              MSH(3) = MSG(3)
          ELSE IF(NVP.EQ.2)THEN
              MSH(2) = MSG(4)
              MSH(3) = MSG(5)
          END IF
C
          IF(NPF.EQ.1)THEN
              MSH(4) = MSG(6)
          ELSE IF(NPF.EQ.2)THEN
              MSH(4) = MSG(7)
              MSH(5) = MSG(8)
          END IF
      END IF
С
С
      CHECK TO SEE IF NPF SHOULD BE OVERRIDDEN; IF SO, REWRITE MESSAGES
С
      I = 0
      IF(VIBL.GT.0.0)I = 1
С
      IF(B2.EQ.'N'.AND.NPF.EQ.1)THEN
          MSH(3+I) = MSG(7)
          MSH(4+I) = MSG(8)
      ELSE IF(B2.EQ.'T'.AND.NPF.EQ.2)THEN
          NPF = 1
          MSH(3+I) = MSG(6)
          MSH(4+I) = '
```

```
END IF
C
С
      CHECK TO SEE IF NVP SHOULD BE OVERRIDDEN; IF SO, REWRITE MESSAGES
С
      IF(B1.EQ.'N'.AND.NVP.EQ.1)THEN
          NVP = 2
          MSH(1+I) = MSG(4)
          MSH(2+I) = MSG(5)
      ELSE IF(Bl.EQ.'T'.AND.NVP.EQ.2)THEN
          NVP = 1
          MSH(1+I) = MSG(1+I)
          MSH(2+I) = MSG(3)
      END IF
С
      CHECK THE LTE FLAG
      IF(COD.EQ.'LTE'.AND.NVP.NE.3)THEN
          NPF = 3
          NVP = NVP + 2
          IF(VIBL.GT.0.0)NVP = 3
      END IF
C
C
      SET INDEX
С
      INDEX = 1
      IF(VIBL.GT.0.0)INDEX = 7
      IF(NPF.EQ.2)INDEX = INDEX + 1
      IF(NVP.EQ.2)INDEX = INDEX + 2
      IF(NPF.EQ.0)INDEX = NVP + 4
      IF(NPF.EQ.3)INDEX = NVP + 8
      WRITE OUT THE DIAGNOSTIC MESSAGES TO UNIT 6
С
С
      WRITE(6,100)(MSH(I),I=1,5),CODE
      RETURN
      END
```

.3682493515461E-43,

.6205657919638E-48,

.8373419683872E-53,

.9186429502399E-58,

.8304614505929E-63,

.6259184116949E-68,

C

Ε

F

```
VOIGT PROFILE ALGORITHM DESIGNED FOR FAST EXECUTION IN FROGRAM NUTE.
     DOPPLER PROFILE IS SUBSTITUTED IN SOME REGIONS. THE METHOD EMPLOYED
      IN REGIONS 1, 2 AND 3 WAS ORIGINALLY CUTLINED BY PIERLUISSI ET AL,
      JQSRT 18, 555(1977). THE ROUTINE HAS BEEN TESTED FOR 0 < X < 25 AND Y=0,
      .000001<Y<10. IT GIVES AN ACCURACY OF BETTER THAN .1% FOR X<1.25 AND
      BETTER THAN .5% EVERYWHERE ELSE IN THIS AREA. THAT IS, THE ABSOLUTE
     ERROR IS LESS THAN .001 OR .005 TIMES THE CORRECT FUNCTION VALUE.
      FOR Y<.000001, WHERE THE DOPPLER PROFILE IS SUBSTITUTED,
                                                                  THE FRAC-
      TIONAL ERROR MAY BE GREATER FOR X>3.3 BUT THE ABSOLUTE ERROR IS VERY
     SMALL.
     THE SUBROUTINE FORM OF ZVGTC IS SET UP TO EVALUATE AN ARRAY OF VOIGT
     FUNCTIONS, VGT, CORRESPONDING TO A SINGLE FREQUENCY DV AND DIFFERENT ALTITUDES. THE INPUT COMING THROUGH COMMON /C/ INCLUDES ARRAYS SPEC-
     IFYING THE LINEWIDTH RATIO AND THE DOPPLER WIDTH FOR EACH ALTITUDE.
     K1 AND K2 ARE THE BOTTOM AND TOP LAYER-INDICES.
     Y = A = SQRT(LN2)*ALFL/ALFD
     X = SQRT(LN2)*DV/ALFD
     DV = NU - NU0
     RAT = ARRAY OF VALUES OF Y
      DWID = ARRAY OF VALUES OF ALFD (DOPPLER WIDTHS)
      VGT = ARRAY OF FUNCTION VALUES
            = 1/(N|*(2N+1)), N = 0,...,56 (COEFFS, REGION 1 SERIES)
            = WEIGHT FOR 2-PT GAUSS-HERMITE QUADRATURE TIMES 2/PI
     W1-W3 = WEIGHTS FOR 6-PT GAUSS-HERMITE QUADRATURE TIMES 2/PI
            = SQUARE OF ZERO
                                FIXED BY 2-PT GAUSS-HERMITE QUADRATURE
      U1-U3 = SQUARES OF ZEROES FIXED BY 6-PT GAUSS-HERMITE QUADRATURE
                            SL = SQRT(LN2);
     PISO = 2/SQRT(PI);
                                              SLP = SQRT(LN2/PI)
      DIMENSION AN(57), TST1(9), TST2(6), RAT(250), DWID(250), VGT(250)
     COMMON/C/RAT, DWID, VGT
      DATA (TST1(N), N=1,9)/4*.90E-03,.17E-03,.32E-04,.62E-05,2*.10E-05/
      DATA (TST2(N), N=1,6)/.10E+00,.10E-01,.10E-02,.10E-03,2*.10E-04/
C
     .10.
       .2380952380952E-01, .4629629629630E-02,
                                                  .7575757575758E-03,
        .1068376068376E-03,
                             .1322751322751E-04,
                                                  .1458916900093E-05,
        .1450385222315E-06,
                             .1312253296380E-07,
                                                  .1089222103715E-08,
       .8350702795147E-10,
                             .5947794013638E-11,
                                                  .3955429516459E-12,
       .2466827010264E-13,
                             .1448326464360E-14,
                                                  .8032735012416E-16,
                             .2107855191442E-18,
                                                  .1002516493491E-19,
        .4221407288807E-17,
                             .1977064753878E-22,
        .4551846758928E-21,
                                                  .8230149299214E-24,
        .3289260349176E-25,
                             .1264107898899E-26,
                                                  .4678483515519E-28,
     8
                             .5754191643982E-31,
                                                  .1916942862110E-32.
        .1669761793417E-29,
                             .1930357208815E-35,
                                                  .5846755007469E-37,
       .6180307588223E-34,
     Α
                                                  .1363041261779E-41,
     В
       .1718856062802E-38,
                             .4908923964523E-40,
```

.9687280238871E-45,

.1513107949541E-49,

.1902541227290E-54,

.1954102582324E-59,

.1660580513451E-64,

.1180761838912E-69,

.2483069097455E-46,

.3601579309810E-51,

.4226789754194E-56,

.4070135277853E-61,

.3255395462013E-66,

.2186210422954E-71,

```
.3974252722665E-73, .7095717391818E-75, .1244665977389E-76/
С
                   /.4697186393498/
      DATA SLP
      DATA PISQ,SL /1.128379167096,
                                      .8325546111577/
      DATA W1,W2,W3/.4613135279626, .09999216171035,.2883893874868E-02/DATA U1,U2,U3/.1901635091935, 1.784492748543, 5.525343742263/
      DATA W6,U6
                  /.5642150484, .5/
C
      ***********************
C
      DO 500 K = K1, K2
      X = DV*SL/DWID(K)
      Y = RAT(K)
С
С
      DETERMINE WHICH REGION TO ENTER
      IF(X.GT.4.9)THEN
          INDEX = 3
      ELSE IF(Y.LT.1.0E-06)THEN
          INDEX = 4
      ELSE IF(Y.GT.1.5)THEN
          INDEX = 2
      ELSE
          INDEX = 1
          N = 1 + INT(3.333333333333*(X-3.3))
          IF(X.LT.3.3) THEN
              N = 1 + INT(2.5*(X-.1))
              IF(Y.LT.TST1(N))INDEX = 4
          ELSE IF(Y.GT.TST2(N))THEN
              INDEX = 2
          END IF
      END IF
С
      ******
C
C
      REGION ONE: PIERLUISSI'S SERIES, EXTENDED
С
C
      IF(INDEX.EQ.1)THEN
          S = X * X - Y * Y
          T = 2.0*X*Y
          SER = Y
          SEI = -X
          FPR = Y
          FPI = -X
C
          NMAX = INT(10.45*X) - 4 + 6*INT(Y)
          N = 8 + 4*INT(Y)
          IF(NMAX.LT.N)NMAX = N
С
          DO 100 N = 1, NMAX
          FNR = FPR*S - FPI*T
          FNI = FPI*S + FPR*T
          SER = SER + FNR*AN(N+1)
          SEI = SEI + FNI*AN(N+1)
          FPR = FNR
  100
          FPI = FNI
          VGT(K) = SLP*EXP(-S)*(COS(T)*(1.0-PISQ*SER) - SIN(T)*PISO*SEI)
C
      *******
C
      REGION TWO: 6-PT GAUSS-HERMITE QUADRATURE
```

```
С
С
       ELSE IF(INDEX.EQ.2)THEN
             S = X * X - Y * Y
             T = 2.0*X*Y
             T2 = T*T
            T = T \star X
            Fl = S - Ul
            F2 = S - U2
F3 = S - U3
            VGT(K) = SLP*(W1*(T - Y*F1)/(F1*F1 + T2) + W2*(T - Y*F2)/(F2*F2 + T2) + W3*(T - Y*F3)/(F3*F3 + T2))
0000
       REGION THREE: 2-PT GAUSS-HERMITE QUADRATURE (FASTER THAN DOPP)
С
       ELSE IF(INDEX.EQ.3)THEN
             T = 2.0*X*Y
             SEI = T*T
            T = T \star X
            FPR = X*X - Y*Y - U6
             VGT(K) = SLP*W6*(T - Y*FPR)/(FPR*FPR + SEI)
С
C
       REGION FOUR: SUBSTITUTE DOPPLER PROFILE
С
            VGT(K) = SLP*EXP(-X*X)
       END IF
  500 \text{ VGT}(K) = \text{VGT}(K)/\text{DWID}(K)
С
C
       RETURN
       END
```

```
SUBROUTINE SPECTRM(VMIN, VMAX, DEL, FWHM, UNIT, MOL, ISC, UST, LST,
     1BR.HGTS.IMXX,LOOK.MSG)
\Gamma
      CHARACTER*1 BL
      CHARACTER*2 BR
      CHARACTER*3 MOL
      CHARACTER*4 UN, UNIT
      CHARACTER*7 FN, LL
      CHARACTER*8 UST, LST
      CHARACTER*10 MSG(2)
      LOGICAL EX, OD, CMPL
      REAL EPS
      PARAMETER (CMPL=.FALSE., EPS=1.0E-06)
      DIMENSION HGTS(50),R(500,12),GL(500),RAW(5),RAI(12)
      SAVE R, GL, RAI, LMAX, IMAX, NOB
  100 FORMAT('CXXXXXXX BAND RADIANCE
                                             ---NLTE OUTPUT')
  101 FORMAT('C',A3,I4,2A8,1X,A2,'---',2A10)
  102 FORMAT(F8.3,F7.3,1X,A4,A7,' LOOK; HTS (KM) =',12F7.2)
  103 FORMAT(F8.3,F7.3,1X,A4,A7,17X,12F7.2)
  104 FORMAT(F10.3,1X,1P,12E10.3)
  105 FORMAT(20X, 15, E10.3)
  106 FORMAT(//,' UNIT 7 HEADER:',/)
  107 FORMAT(1H1, 'SUBROUTINE SPECTRM: ',//,
     1' CUMULATIVE RADIANCE FOR', 13, ' VIEWING PATHS AND', 13, 1X, A3,
     2' BANDS',//,' INTEGRATED RADIANCE (WATT/CM2*STER)',/,
3' SYNTHETIC SPECTRUM (WATT/CM2*STER*',A4,')',//,
     4' FWHM FOR TRIANGULAR SCANNING FUNCTION = ',F7.3,1X,A4,' DEL = ',
     5F6.3,1X,A4)
  108 FORMAT(/,3X,A7,1X,12(F7.2,' KM'))
  109 FORMAT(/,' CREATE NEW DATABASE FOR BAND RADIANCES ON UNIT 7,',
     1' FILE SPECF')
  110 FORMAT(/,' SUBROUTINE SPECTRM RECOGNIZES FILE WITH PREVIOU'
     1'SLY-CALCULATED BAND RADIANCES; WILL ADD TO THIS DATA-BASE',/)
  111 FORMAT(/,' SUBROUTINE SPECTRM DETECTS INCONSISTENCIES BETWEEN',
     1' CURRENT AND PREVIOUS VALUES OF SIGNIFICANT',/,' PARAMETERS,',
     2' WILL MOT ADD BAND RADIANCES; IGNORE PREVIOUS UNIT 7, OPEN',
  3' NEW UNIT 7 AS FILE SPECG')
112 FORMAT(/,' PARAMETER VALUES ARE:
                                           PRESENT PREVIOUS',/,
     1/,17X,'FWHM',2F10.3,
     2/,17X,'DEL ',2F10.3,
3/,17X,'GEOM',2(3X,A7),
     4/,17X, 'UNITS',5X,A4,6X,A4,
  512(/,16X,A1,'ALT ',2F10.2))
113 FORMAT(///,' $$$$ PROBLEM IN ACCESSING UNIT',12,
     1' (INQUIRE), FWHM WILL BE RESET TO ZERO $$$$$',A1,/,
     2', $$$$$ SEE UNIT 6 OUTPUT $$$$$',//)
  114 FORMAT(' IOSTAT =', 16, A1,
     1/,' EX =',L2,
2/,' OD =',L2,
3/,' NM =',I2,
     4/.' FN = '.A7,
     5//, FWHM RESET TO ZERO, CONTINUE WITH NLTE : //)
  115 FORMAT(//,' $$$$$ CAUTION: SPECTRAL RADIANCE ARRAY IS TOO SMALL,',
     1' SOME POINTS ARE NOT CALCULATED $$$$$',/,
        $$$$$',10X,'GMIN, GMAX, DEL =',3F10.3,1X,A4,17X,'$$$$$',//)
  116 FORMAT(F10.3,10E10.3)
  117 FORMAT(' LMAX =',14,'
                                RANGE =',F9.3,' TO',F9.3.2X,A4)
  118 FORMAT(//,' $$$$$ PROBLEM OPENING ',A4,'FILE',A7,'ON UNIT',I2,
```

```
IOS = ', I4, /, 6X, ' RESET FWHM TO ZERO AND CONTINUE WITH NLTE',
  2' $$$$$',//)
119 FORMAT(' NOTE THAT IMAX =',I3,' BUT ONLY 12 SPECTRA ARE WRITTEN',
     1' TO UNIT 7')
  120 FORMAT(I3,8X,1P,12E10.3)
  121 FORMAT(' (INTEG''TD)', 1P, 12E10.3)
С
С
C
С
С
      SUBROUTINE SPECTRM---PURPOSE IS TO GENERATE A SYNTHETIC SPECTRUM FOR
C
      THE VIBRATIONAL BAND UNDER CONSIDERATION AND ADD THE RESULTS TO SPEC-
      TRA FROM OTHER BANDS PREVIOUSLY GENERATED. ONLY 12 L-O-S PATHS CAN BE
С
      CONSIDERED AT ONCE --- OTHERS ARE IGNORED BY THIS ROUTINE.
С
      MAIN ENTRY: CHECK TO SEE IF PREVIOUSLY-GENERATED SPECTRA ARE AVAILA-
C
                   BLE. PERFORM INITIALIZATION STEPS, OPEN UNIT 7, AND READ
                   PREVIOUS RESULTS (IF ANY).
C
      ENTRY SPEC1: ADD THE CONTRIBUTIONS FOR EACH LINE-OF-SIGHT PATH (I) AT
C
                   EACH DESIGNATED WAVELENGTH (L)
С
      ENTRY SPEC2: ADD THE CONTRIBUTIONS FROM THE CURRENT BAND TO THE RE-
C
                   SULTS FROM BANDS COMPILED EARLIER (IF ANY). WRITE THE
                   RESULTS TO UNIT 7.
С
C
        **************************
C
С
      MAIN ENTRY:
C
      INITIALIZATION
      BL = ' '
      IMAX = IMXX
      IF(IMAX.GT.12)IMAX = 12
C
      UNITS CHOSEN ARE EITHER CM-1 OR UM (MICRONS)
¢
      VMIN, VMAX ARE IN CM-1, HOWEVER.
      IF (UNIT. EQ. 'CM-1') THEN
          GMIN = INT((VMIN-FWHM)/DEL)*DEL + DEL
          GMAX = INT((VMAX+FWHM)/DEL)*DEL
      ELSE
          GMAX = 10000./VMIN + FWHM
          GMIN = 10000./VMAX - FWHM
          GMIN = INT(GMIN/DEL)*DEL + DEL
          GMAX = INT(GMAX/DEL)*DEL
      END IF
С
      QUERY BY FILENAME TO ESTABLISH THE CURRENT STATUS OF SPECF
      L1 = 7
      LL = ' SPECF '
      UN = 'OLD '
      INQUIRE(FILE='SPECF', IOSTAT=IOS, ERR=900, EXIST=EX, OPENED=OD,
     lnumber=nm, name=fn)
     FN = ' LIMB'
      IF(LOOK.EQ.1)FN = ' ZENITH'
```

```
IF(.NOT.EX)GO TO 300
С
C
      FILE SPECF EXISTS AS A LOCAL FILE; READ IT
C
      OPEN(7, IOSTAT=IOS, ERR=901, FILE='SPECF', STATUS='OLD')
      REWIND(7)
      WRITE(4,106)
      IF(CMPL)
C$
      WRITE(9,106)
      ENDIF
CS
      CALL HEADER(7)
      READ(7,103)FW,DL,UN,LL,(GL(I),I=1,IMAX)
      READ(7,120)NOB,(RAI(I),I=1,IMAX)
С
      PARAMETER CHECK (VALUES ON THE FIRST DATA CARD-IMAGE)
      TEST = ABS(FWHM-FW)
      V = ABS(DEL-DL)
      IF(TEST.GT.EPS.OR.V.GT.EPS)GO TO 290
      IF(FN.NE.LL.OR.UNIT.NE.UN)GO TO 290
      DO 210 I = 1,IMAX
      V = ABS(GL(I)-HGTS(I))
  210 IF(V.GT.EPS)GO TO 290
      WRITE(4,110)
      IF(IMXX.GT.IMAX)WRITE(4,119)IMXX
C$
      IF(CMPL)
      WRITE(9,110)
C$
      ENDIF
С
      PARAMETERS CHECK OUT: READ THE PREVIOUSLY-COMPILED BAND-RADIANCE DATA
C
      DO 220 L = 1,500
      READ(7,104,END=225)GL(L),(R(L,I),I=1,IMAX)
  220 LMAX = L
  225 CONTINUE
      WRITE(4,117)LMAX,GL(1),GL(LMAX),UNIT
      IF NECESSARY, ADJUST THE INDEX RANGE (1-LMAX) TO COVER THE FULL WAVE-
С
      LENGTH OR ENERGY RANGE (GL(1)-GL(LMAX)) REQUIRED BY THE CURRENT BAND AND THE ONES PREVIOUSLY COMPILED. IF MORE THAN 500 POINTS ARE REQUES-
С
      TED, ELIMINATE SOME NEW POINTS RATHER THAN THOSE FROM EARLIER BANDS.
С
      K = INT((GL(1)-GMIN)/DEL + EPS)
      IF(K.GT.0.AND.LMAX.LT.500)THEN
          IF((K+LMAX).GT.500)THEN
               K = 500 - LMAX
               WRITE(4,115)GMIN,GMAX,DEL,UNIT
               WRITE(6,115)GMIN,GMAX,DEL,UNIT
          END IF
          DO 230 L = LMAX, 1, -1
          GL(L+K) = GL(L)
          DO 230 I = 1, IMAX
          R(L+K,I) = R(L,I)
  230
          DO 235 L = 1, K
          GL(L) = GL(K+1) - (K-L+1)*DEL
          DO 235 I = 1,IMAX
```

```
235
          R(L,I) = 0.0
          LMAX = LMAX + K
      END IF
C
      K = INT((GMAX-GL(LMAX))/DEL + EPS)
      IF(K.GT.O.AND.LMAX.LT.500)THEN
          IF((K+LMAX).GT.500)THEN
              K = 500 - LMAX
              WRITE(4,115)GMIN,GMAX,DEL,UNIT
             WRITE(6,115)GMIN,GMAX,DEL,UNIT
          END IF
          DO 245 L = LMAX+1,LMAX+K
          GL(L) = GL(LMAX) + (L-LMAX)*DEL
          DO 245 I = 1,IMAX
  245
         R(L,I) = 0.0
          LMAX = LMAX + K
      END IF
      WRITE(4,117)LMAX,GL(1),GL(LMAX),UNIT
C
С
      REPOSITION UNIT 7, RETURN TO LINES
C
      CALL REWND(7)
      WRITE(7,101)MOL, ISO, UST, LST, BR, MSG(1), MSG(2)
      WRITE(7,102)FWHM, DEL, UNIT, FN, (HGTS(I), I=1, IMAX)
      RETURN
C
      ***********
С
C
C
      PARAMETERS DON'T CHECK OUT: FILE SPECF CONTAINS THE WRONG INFORMATION
      OPEN SPECG AS AN ALTERNATE FILE FOR OUTPUT FROM THE CURRENT BAND.
C
  290 WRITE(4,111)
      WRITE(6,111)
C$
      IF(CMPL)
      WRITE(9,111)
C$
     WRITE(4,112) FWHM, FW, DEL, DL, FN, LL, UNIT, UN, (BL, HGTS(I), GL(I),
     li=1,IMAX)
     WRITE(6,112)FWHM,FW,DEL,DL,FN,LL,UNIT,UN,(BL,HGTS(I),GL(I),
     lI=1, IMAX)
     CLOSE(7)
     LL = ' SPECG '
     UN = 'NEW
     OPEN(7, IOSTAT=IOS, ERR=901, FILE='SPECG', STATUS='NEW')
     GO TO 301
С
      ***********
С
С
С
     FILE SPECF DOES NOT EXIST OR IS EMPTY; OPEN IT AS UNIT 7. WRITE HEAD-
С
     ERS AND THE INITIAL DATA RECORD.
  300 LL = ' SPECF '
     UN = 'NEW
     OPEN(7, IOSTAT=IOS, ERR=901, FILE='SPECF', STATUS='NEW')
     WRITE(4,109)
CS
     IF(CMPL)
     WRITE(9,109)
     ENDIF
  301 IF(IMXX.GT.IMAX)WRITE(4,119)IMXX
     WRITE(7,100)
```

```
WRITE(7,101)MOL,ISC,UST,LST,BR,MSG(1),MSG(2)
     WRITE(7,102) FWHM, DEL, UNIT, FN, (HGTS(I), I=1, IMAX)
     DEFINE THE ARRAY OF WAVENUMBERS OR WAVELENGTHS TO BE USED. INITIALIZE
     THE ARRAY OF SPECTRAL INTENSITIES AND THE TOTAL INTEGRATED RADIANCE
     ARRAY FOR EACH LINE-OF-SIGHT PATH. RETURN TO LINES.
     0 = 400
     DO 355 I = 1, IMAX
 355 RAI(I) = 0.0
     50.360 L = 1,500
     GL \cdot L) = GMIN + DEL*(L-1)
     IF(GL(L).GT.(GMAX+EPS))GO TO 370
     LMAX = L
     DO 360 I = 1, IMAX
 360 R(L,I) = 0.0
     IF: (GL(500) +DEL).LT.GMAX)THEN
        WRITE, 4,115) GMIN, GMAX, DEL, UNIT
        WRITE(6,115)GMIN,GMAX,DEL,UNIT
     END IF
 370 WRITE(4,117)LMAX,GL(1),GL(LMAX),UNIT
     RETURN
C
     *******
     ************
C
     ENTRY SPEC1: ADD THE CONTRIBUTION FROM THE CURRENT LINE TO THE CUMU-
C
     LATIVE RESULTS OBTAINED SO FAR.
C
C
     ENTRY SPEC1 (FWHM, VINIT, NR, IMXXX, RAW)
С
     FW = FWHM*FWHM
     V = VINIT
     IF(UNIT.NE.'CM-1')V = 10000./VINIT
     NM = IMXXX
     K = 5*(NR-1) + IMXXX
     IF(K.GT.12)NM = 2
С
     DO 400 L = 1, LMAX
     TEST = ABS(GL(L)-V)
     IF(TEST.GT.FWHM)GO TO 400
     DO 395 I = 1,NM
     K = 5*(NR-1) + I
 395 R(L,K) = R(L,K) + RAW(I)*(FWHM-TEST)/FW
 400 CONTINUE
     DO 410 I = 1, NM
     K = 5*(NR-1) + I
 410 \text{ RAI}(K) = \text{RAI}(K) + \text{RAW}(I)
     RETURN
С
     *********
     ********
C
     ENTRY SPEC2: WRITE THE COMPLETED SYNTHETIC SPECTRUM TO UNITS 4 AND 7
C
     ENTRY SPEC2(FWHM)
     NOB = NOB + 1
     FN = '(CM-1)'
```

```
IF(UNIT.NE.'CM-1')FN = ' WL(UM)'
WRITE(4,107)IMAX,NOB,MOL,UNIT,FWHM,UNIT,DEL,UNIT
      WRITE(4,108) FN, (HGTS(I), I=1, IMAX)
      WRITE(4,102)
      WRITE(7,120)NOB,(RAI(I),I=1,IMAX)
      WRITE(4,121)(RAI(I), I=1, IMAX)
      WRITE(4,102)
      DO 500 L = 1,LMAX
      WRITE(7,104)GL(L),(R(L,I),I=1,IMAX)
  500 WRITE(4,104)GL(L),(R(L,I),I=1,IMAX)
      REWIND(7)
      CLOSE(7)
      RETURN
0000000
      ERROR RETURNS: THERE IS A PROBLEM WITH AN INQUIRE OR OPEN
  900 WRITE(4,113)L1,BL
      WRITE(6,113)L1
      WRITE(6,114)IOS, BL, EX, OD, NM, FN
      FWHM = 0.0
      RETURN
С
  901 WRITE(4,118)UN, LL, L1, IOS
      WRITE(6,118)UN,LL,L1,IOS
      FWHM = 0.0
      RETURN
      END
```

```
SUBROUTINE PATH(ALT, HGTS, IMXX, HTS, IMAX, NR, KMAX, LOOK, K1)
000
      SUBROUTINE TO SET THE LOWER-ALTITUDE INDEX, K1, FOR EACH L-O-S PATH
      AND TO PRINT THE PARAMETERS DESCRIBING THE PATHS.
      CHARACTER*9 MSG(2)
      DIMENSION ALT(250), HGTS(50), HTS(5), K1(5)
      DATA MSG(1), MSG(2)/', TANGENT',', OBSERV.'/
      DETERMINE IMAX AND STACK THE VALUES OF HGTS INTO HTS
      K = IMXX - 5*(NR-1)
      IMAX = MIN(K,5)
      DO 170 I = 1, IMAX
K = 5*(NR-1) + I
  170 HTS(I) = HGTS(K)
      WRITE(4,101)NR, IMAX
000
      SET KI FOR EACH PATH
      DO 200 I = 1, IMAX
      DO 180 K = 1, KMAX-1
      IF(ALT(K+1).GT.HTS(I))THEN
         Kl(I) = K
         GO TÓ 190
      END IF
  180 CONTINUE
      IF(ALT(KMAX), LE, HTS(I))Kl(I) = KMAX
      WRITE THE PATH PARAMETERS
  190 J = KMAX - K1(I) + 1
     K = 5*(NR-1) + I
  200 WRITE(4,100)K,MSG(LOOK+1),HTS(I),K1(I),KMAX,ALT(K1(I)),ALT(KMAX),J
C
 C
     RETURN
     END
```

```
SUBROUTINE HEADER(IU)
С
     SUBROUTINE TO READ THE HEADERS ON THE INPUT FILES USED, AND TO COPY
C
     THEM, FOR REFERENCE, TO UNIT 6. IU IS THE UNIT NUMBER.
С
     CHARACTER*1 CH, BL
     CHARACTER*130 MSG
     DIMENSION NU(7)
     SAVE NU
С
 100 FORMAT(A1,A120)
 1'FFFFFFFFFFFGGGGGGGGGGGG------,33X,'(FORMAT)')
 1'666666666677777777788888888888',43%,'(FORMAT)')
 105 FORMAT(1X,A1,A120,' (DATA)')
С
     BL = ' '
     J = 0
     WRITE(6,102)IU
 200 READ(IU, 100)CH, MSG
     IF(CH.EQ.'C')THEN
        WRITE(4,100)BL,MSG
        WRITE(9,100)BL,MSG
        WRITE(6,101)CH,MSG
        J = J + 1
GO TO 200
     ELSE
        BACKSPACE IU
        IF(IU.EQ.2)WRITE(6,103)
        IF(IU.NE.2)WRITE(6,104)
        WRITE(6,105)CH,MSG
        NU(IU) = J
     END IF
     RETURN
С
     ENTRY REWND(IU)
C
C
     PROCEDURE TO REPOSITION THE INPUT FILES AT THE FIRST DATA CARD-IMAGE
Ċ
     (E.G., SKIP THE HEADER)
C
     REWIND(IU)
     IF(NU(IU).EQ.0)RETURN
     DO 300 J = 1,NU(IU)
 300 READ(IU,100)CH
     RETURN
     END
```

```
FUNCTION VWERF (XX,A)
      THE METHOD IS DUE TO RYBICKI. THE FORTRAN LISTING WAS
C
      PUBLISHED AS AN APPENDIX TO E. H. AVRETT AND R. LOESER, "FORMATION OF LINE AND CONTINUOUS SPECTRA," SPECIAL REPORT 303,
C
      SMITHSONIAN ASTROPHYSICAL OBSERVATORY, CAMBRIDGE, MASS. (1970)
С
C
C
      THE METHOD OF CALCULATION IS DESCRIBED BY B. H. ARMSTRONG
      AND R. W. NICHOLLS, "EMISSION, ABSORPTION AND TRANSFER OF
С
      RADIATION IN HEATED ATMOSPHERES," PERGAMON PRESS, NEW YORK,
C
      (1972) - PP. 235-237.
C
C
C
      "ORIGINAL" VERSION FROM DEGGES CHANGED BY ADDITION OF SAVE STATEMENT
       COMPLEX Z
       DIMENSION C(131)
      SAVE NTRY, NP1, NPNP1, RHSQ, Q1, RTLN2, C
       DATA NTRY, NMAX, RH, PI, Q2, Q3 /1, 15, 3.0, 3.1415, 26535898,
     1 5.6418958354776E-01,8.9793561062583E-02/
C
       IF (NTRY .EQ. 1) GO TO 170
  110 CONTINUE
       X = RTLN2*XX
       IF (A .EQ. 0.0) GO TO 160
       IF ((X + A) .GT. 25.0) GO TO 190
      DO COMPUTATION FOR GENERAL CASE
       A1 = RH*A
       A2 = A*A
       IF (A .LT. 0.1) GO TO 120
       Z = CEXP(CMPLX(-Q1*A,Q1*X))
       VWERF = 0.0
       GO TO 130
  120
      CONTINUE
       Z = CCOS(CMPLX(Q1*X,Q1*A))
       VWERF = Q2*EXP(A2 - X*X)*COS(2.0*A*X)
  130 CONTINUE
       B1 = (1.0 - REAL(Z))*A*0.5*RH
       B2 = -AIMAG(Z)
       S = -0.5*(FLOAT(NP1) + RH*X)
       T = S*S + 0.25*RHSQ*A2
      DO 150 N = 1, NPNP1
       T = T + S + 0.25
       S = S + 0.5
       B1 = A1 - B1
       B2 = -B2
       IF (T .GT. 2.5E-12) GO TO 140
       VWERF = VWERF - C(N)*A/RH
       GO TO 150
  140 CONTINUE
       VWERF = VWERF + C(N)*(B2*S + B1)/T
  150
      CONTINUE
  155 CONTINUE
       VWERF = VWERF*RTLN2
       RETURN
  160
      CONTINUE
       VWERF = RTLN2*Q2*EXP(-X*X)
       RETURN
  170 CONTINUE
       NTRY = 0
```

```
NP1 = NMAX + 1
       NPNP1 = NMAX + NP1
       RHSQ = RH*RH
       K = -NP1
      DO 180 N = 1, NPNP1
       K = K + 1
       C(N) = Q3*EXP(-FLOAT(K*K)/RHSQ)
  180 CONTINUE
       Q1 = RH*PI
       RTLN2 = SQRT(ALOG(2.0))
       GO TO 110
  190 CONTINUE
      USE ASYMPTOTIC EXPANSION FOR COMPLEX ERROR FUNCTION
      FOR LARGE X AND A.
С
Ċ
       AN = 2.5
       DENR = A
      DENI = -X
DO 200 I = 1, 5
       DEN = AN/(DENR*DENR + DENI*DENI)
       DENR = DEN*DENR + A
       DENI = -DENI*DEN - X
       AN = AN - 0.5
  200 CONTINUE
       DEN = Q2/(DENR*DENR + DENI*DENI)
VWERF = RTLN2*Q2*DEN*DENR
       RETURN
      END
```

```
SUBROUTINE MOLEC(MOL, ISO, UST, LST, MOLWT, DEGV, PROT, TEXP, VIBE, VIBL,
                      VIBQ,GL,GU,AI,FMT,FLAG)
      **********
C
      SUBROUTINE MOLEC, GIVEN THE MOLECULE CODE (MOL) AND THE ISOTOPE CODE
      (ISO), RETURNS PARAMETERS WHICH ARE UNIQUELY ASSOCIATED WITH THE MOL-
      ECULE IN QUESTION:
                          MOLWT, THE MOLECULAR WEIGHT
                                THE DEGENERACY OF THE VIBRATIONAL MANIFOLD
                          DEGV,
                                 THE EXPONENT OF TEMPERATURE IN THE ROTAT'L
                          PROT,
                                 PARTITION FUNCTION
C
                                THE EXPONENT OF TEMPERATURE IN THE LORENTZ
C
                          TEXP.
                                 LINEWIDTH CORRECTION
                         VIBQ,
                                THE VIBRATIONAL QUANTUM IN THE PARTIT'N FN
C
                          AI.
                                THE ISOTOPIC ABUNDANCE
     ALSO, MOLEC RETURNS A CHARACTER VARIABLE, FMT, SPECIFYING THE FORMAT
     NEEDED FOR READING THE LINEFILES. SINCE BR AND NRL (SEE LINES) ARE
     NOT APPROPRIATE DESCRIPTIONS FOR H2O, O3, AND CH4 (THE NONLINEAR MOL-
     ECULES), THE LINES ARE SIMPLY NUMBERED IN THE ORDER IN WHICH THEY ARE
C
     READ.
C
С
     FOR CH4, THE CORRECT PARTITION FUNCTION RESULTS TO WITHIN ONE PERCENT
     IF A SINGLE LEVEL AT 1370 CM-1 (VIBQ) WITH A DEGENERACY OF 5 (DEGV)
C
     IS CHOSEN.
C
     DEGV IS 2 FOR LINEAR TRIATOMIC MOLECULES, 5 FOR CH4, 1 OTHERWISE
C
     PROT IS 1 FOR ALL LINEAR MOLECULES, 1.5 OTHERWISE
     TEXP IS .25 FOR CO2, .5 OTHERWISE
C
     GIVEN THE UPPER AND LOWER VIBRATIONAL LEVEL CODES (UST AND LST), THIS
     SUBROUTINE ALSO RETURNS CERTAIN VALUES WHICH ARE ASSOCIATED
                                                                      WITH
     INDIVIDUAL VIBRATIONAL TRANSITIONS, PROVIDED THE LATTER CAN BE FOUND
C
C
     IN THE DATABASE MOLPAR. MOLPAR CONTAINS DATA PERTAINING ONLY TO TRAN-
     SITIONS OF CO2 AND NO, AND NOT ALL TRANSITIONS AT THAT. THE INTEGER
     VARIABLE FLAG IS SET TO ZERO IF THESE QUANTITIES ARE NOT FOUND.
C
     THIS SUBROUTINE, AND HENCE PROGRAM NLTE, RECOGNIZES ONLY THE FIRST
     EIGHT MOLECULES IN THE A.F.G.L. DATABASE --- THAT IS, ONLY THOSE WHOSE
     CODES APPEAR IN THE FIRST DATA STATEMENT BELOW.
     INTEGER DEGV,DEG(8),STW2(29),STW8(13),GL,GU
     LOGICAL FLAG
     CHARACTER*3 MOLCOD(8), MOL
     CHARACTER*8 NAM2(29), NAM8(13), UST, LST
     CHARACTER*31 F1
     CHARACTER*9 F2
     CHARACTER*7 F3
     CHARACTER*47 FMT
     DIMENSION ENL2(29,7), ENL8(13,3)
     DIMENSION MLWT(8,7), MISO(8,7), ABUN(8,7), VIB(8,7), PRT(8), TXP(8)
     COMMON/M/MISO, MLWT, ABUN, VIB, DEG, PRT, TXP, ENL2, STW2, ENL8, STW8
     COMMON/N/NAM2, NAM8
     DATA (MOLCOD(I), I=1,8)/'H2O', 'CO2', 'O3 ', 'N2O'. 'CO ', 'CH4', 'O2 '.
                            'NO '/
```

DATA F1/'(BZ,F10.4,E10.3,F5.4,F10.3,2A8,'/

```
DATA F3/',4X,I4)'/
С
   90 FORMAT(//,' $$$$$ ERROR: MOLECULE OR ISOTOPE CODE NOT RECOG',
     1'NIZED $$$$$',/)
С
С
      CHECK THE MOLECULE AND ISOTOPE CODES
      IC = 0
      DO 100 I = 1.8
  100 IF(MOLCOD(I).EQ.MOL)IC = I
      IF(IC.EQ.0)THEN
          WRITE(4,90)
          WRITE(6,90)
          RETURN
      END IF
      ID = 0
      DO 110 I = 1,7
  110 IF(MISO(IC,I).EQ.ISO)ID = I
      IF(ID.EQ.0)THEN
          WRITE(4,90)
          WRITE(6,90)
          RETURN
      END IF
С
С
      SET THE SIX MOLECULAR PARAMETERS
      MOLWT = MLWT(IC, ID)
      AI = ABUN(IC,ID)
      VIBO = VIB(IC, ID)
      DEGV = DEG(IC)
      PROT = PRT(IC)
      TEXP = TXP(IC)
С
С
      SET THE FORMAT FOR READING THE AFGL LINEFILE.
      F2 = '14X,A1,I3'
      IF(IC.EQ.7)F2 = '12X,A2,I4'
      IF(IC.EQ.1.OR.IC.EQ.3)F2 = 'A1,I17
      IF(IC.EQ.6)F2 = 'A1,16X,I1'
      IF(IC.EQ.8.OR.IC.EQ.5) THEN
          F2 = '12X,A1,I3'
          F3 = ', 6X, I4)'
      END IF
      FMT = F1//F2//F3
С
C
      CHECK TO SEE IF THE PROPERTIES OF THE VIBRATIONAL LEVELS ARE STORED
      IN THE DATABASE, MOLPAR. SET THE INTEGER VARIABLE, FLAG.
С
С
      FLAG = .TRUE.
      IF(IC.EQ.2.OR.IC.EQ.8) THEN
          IMAX = 29
          IF(IC.EQ.8)THEN
              IMAX = 13
              DO 200 I = 1,IMAX
              NAM2(I) = NAM8(I)
              STW2(I) = STW8(I)
  200
              ENL2(I,ID) = ENL8(I,ID)
          END IF
С
          IL = 0
```

```
SUBROUTINE SHFT (VAR, DUM)
С
Ċ
      SUBROUTINE TO CONVERT A LEFT-JUSTIFIED CHARACTER VARIABLE, VAR, TO A
С
      RIGHT-JUSTIFIED VARIABLE.
      CHARACTER VAR*(*), DUM*(*), B*1, BL*1
      DATA BL/' '/
      L = LEN(VAR)
      DO 10 I = 1,L
      B = VAR(L:L)
      IF(B.NE.BL)RETURN
      DUM = BL//VAR
   10 VAR = DUM
      RETURN
      END
      SUBROUTINE LINT(Z,F,F1,F2,Z1,Z2)
С
C
      SUBROUTINE TO PERFORM LINEAR INTERPOLATION OF F(Z)---TO OBTAIN
      F AT A POINT Z.
      D = Z2 - Z1
      F = F2*(Z - Z1)/D - F1*(Z - Z2)/D
      RETURN
      END
      SUBROUTINE VIBTMP(C2, HMIN, HMAX, E, G, POPO, POP1, VT)
C
      SUBROUTINE TO CALCULATE A VIBRATIONAL TEMPERATURE PROFILE FROM TWO
      VIBRATIONAL POPULATION PROFILES. THE LOWER STATE (OF THE TWO WHOSE
C
      POPULATIONS ARE GIVEN) IS ASSUMED TO BE THE GROUND STATE.
С
      INTEGER A, HMIN, HMAX, G
      DIMENSION VT(250), POP0(250), POP1(250)
С
      DO 100 A = HMIN, HMAX
  100 VT(A) = -C2*E/ALOG(POP1(A)/(G*POP0(A)))
      RETURN
      END
      SUBROUTINE VIBPOP(C2, HMIN, HMAX, AI, E, G, RHO, QV, VT, POP)
С
C
      SUBROUTINE TO CALCULATE A VIBRATIONAL POPULATION PROFILE FROM
      THE CORRESPONDING VIBRATIONAL TEMPERATURE PROFILE.
С
      INTEGER A, HMIN, HMAX, G
C
      DIMENSION VT(250), RHO(250), POP(250), QV(250)
      DO 100 A = HMIN, HMAX
  100 POP(A) = AI*G*RHO(A)*EXP(-C2*E/VT(A))/QV(A)
      RETURN
      END
```

```
BLOCK DATA MOLPAR
С
      INTEGER DEGV(8),STW2(29),STW8(13)
      CHARACTER*8 NAM2(29), NAM8(13)
      DIMENSION ENL2(29,7), ENL8(13,3)
      DIMENSION MISO(8,7), MLWT(8,7), ABUN(8,7), VIBQ(8,7), PROT(8), TEXP(8)
      COMMON/M/MISO, MLWT, ABUN, VIBQ, DEGV, PROT, TEXP, ENL2, STW2, ENL8, STW8
      COMMON/N/NAM2, NAM8
С
C
      SET MOLECULAR PARAMETERS FOR H2O
      DATA (MISO(1,I),I=1,7)/161,162,181,171,3*-1/
      DATA (MLWT(1,I),I=1,4)/18, 19, 20, 19/
      DATA (ABUN(1,I),I=1,4)/.99729,.00030,.00204,.00037/
      DATA (VIBQ(1,I),I=1,4)/1594.7498,14J3.489,1588.279,1591.325/
С
      SET MOLECULAR PARAMETERS FOR CO2 (MOLECULE # 2)
С
      DATA (MISO(2,I),I=1,7)/626,636,628,627,638,637,828/
      DATA (MLWT(2,I),I=1,7)/ 44, 45, 46, 45, 47, 46, 48/
      DATA (ABUN(2,I),I=1,7)/.98414,.01105,.00402,.00073,.0000452,
                              .0000082,.00000412/
      DATA (VIBQ(2,1),I=1,7)/667.379,648.479,662.374,664.730,643.23,
                              645.72, 657.33/
С
      SET MOLECULAR PARAMETERS FOR O3
С
C
      DATA (MISO(3,I),I=1,7)/666,668,686,4*-1/
      DATA (MLWT(3,I),I=1,3)/48,50,50/
      DATA (ABUN(3,I),I=1,3)/.99279,.00406,.00203/
      DATA (VIBQ(3,I), I=1,3)/3*700.9316/
C
С
      SET MOLECULAR PARAMETERS FOR N2O
С
      DATA (MISO(4,I),I=1,7)/446,456,546,448,447,2*-1/
      DATA (MLWT(4,I),I=1,5)/ 44, 45, 45, 46, 45/
      DATA (ABUN(4,1), I=1,5)/.99022,.00368,.00368,.00202,.00037/
      DATA (VIBQ(4,I),I=1,5)/588.768,575.5,585.32,584.1,586.3/
C
      SET MOLECULAR PARAMETERS FOR CO
C
      DATA (MISO(5,I),I=1,7)/26,36,28,27,3*-1/
      DATA (MLWT(5,I),I=1,4)/28,29,30,29/
      DATA (ABUN(5,I),I=1,4)/.98652,.01107,.00202,.000369/
      DATA (VIBQ(5,I),I=1,4)/2143.2716,2096.0674,2092.1231,2116.2957/
C
С
      SET MOLECULAR PARAMETERS FOR CH4 (211 AND 311) AND CH3D (212)
      DATA (MISO(6,I),I=1,7)/211,311,212,4*-1/
      DATA (MLWT(6,I),I=1,3)/16, 17, 17/
      DATA (ABUN(6,I,,I=1,3)/.98515,.01110,.00060/
      DATA (VIBQ(6,I), I=1,3)/3*1370./
      SET MOLECULAR PARAMETERS FOR 02
      DATA (MISO(7,I),I=1,7)/66,68,67,4*-1/
      DATA (MLWT(7,I), I=1,3)/32,34,33/
      DATA (ABUN(7,I),I=1,3)/.99519,.00407,.00074/
      DATA (VIBQ(7,I),I=1,3)/3*1556.3791/
```

```
C
Ç
       SET MOLECULAR PARAMETERS FOR NO (MOLECULE # 8)
С
       DATA (MISO(8,I),I=1,7)/46,56,48,4*-1/
       DATA (MLWT(8,I),I=1,3)/30,31,32/
       DATA (ABUN(8,I),I=1,3)/.99390,.00369,.00203/
       DATA (VIBQ(8,I),I=1,3)/1875.9711,1842.9177,1827.2844/
C
C
       SET DEGV, PROT, AND TEXP FOR ALL EIGHT MOLECULES
C
       DATA (DEGV(I), I=1,8)/1,2,1,2,1,5,1,1/
       DATA (PROT(I), I=1,8)/1.5,1.0,1.5,1.0,1.0,1.5,1.0,1.0/
       DATA (TEXP(I), I=1,8)/.5,.25,6*.5/
С
С
Č
                                  CO2 VIBRATIONAL LEVEL PARAMETERS
C
С
       IDENTIFY CO2 ENERGY LEVELS USING AFGL NOTATION
       DATA (NAM2(I),I=1,29)/'00001','01101','10002','02201','10001',
'11102','03301','11101','00011','20003',
'12202','20002','04401','12201','20001',
      2
                                   '01111',
'10012','02211','10011',
'11112','03311','11111','00021',
'20013','12212',
      3
      4
      5
      6
                                   '04411','20012','12211','20011'/
С
С
       SET ENERGY LEVELS FOR THE 626 ISOTOPE
       DATA (ENL2(I,1), I=1,29)/0.,667.379, 1285.4087,1335.129, 1388.1847,
                           1932.472, 2003.244, 2076.855, 2349.1433,2548.373,
                           2585.032, 2671.146, 2671.716, 2760.735, 2797.140,
      2
                           3004.012,
      3
      4
                           3612.842, 3659.271, 3714.783,
                           4247.707, 4314.912, 4390.627, 4673.327, 4853.629, 4887.982,
      5
                           4970.930, 4977.839, 5061.788, 5099.663/
С
C
       SET ENERGY LEVELS FOR THE 636 ISOTOPE
С
       DATA (ENL2(I,2),I=1,29)/0.,648.479, 1265.8282,1297.268, 1370.0625, 1896.547, 1946.343, 2037.093, 2283.4875,2507.50,
      2
                           2531.63, 2595.614, 2645.086, 2700.25, 2750.48,
                           2920.239,
      3
      4
                           3527.7376,3557.316, 3632.9096,
                           4147.239, 4194.704, 4287.70, 4543.549, 4748.062, 4770.987, 4831.99, 4887.387, 4938.802, 4991.346/
      5
      6
С
С
       SET ENERGY LEVELS FOR THE 628 ISOTOPE
       DATA (ENL2(I,3),I=1,29)/0.,662.3743,1259.426, 1325.15, 1365.844, 1901.748, 1988.328, 2049.346, 2332.1127,2500.776,
                           2549.425, 2614.235, 2651.875, 2728.264, 2757.229,
      2
      3
                           2982.106,
                           3571.143, 3632.52, 2675.13,
      5
                           4201.19, 4283.35,
                                                   4346.13, 4639.502,
                           4791.26, 4836.63,
      6
```

```
7
                       4904.846, 4934.565, 5012.55, 5042.584/
C
      SET ENERGY LEVELS FOR THE 627 ISOTOPE
С
      DATA (ENL2(I,4),I=1,29)/0.,664.73,
                                             1271.875, 1329.87, 1376.03,
                       1916.31, 1995.36,
                                             2062.41, 2340.0136,2523.58,
                                  2641.26,
     2
                       2566.33,
                                                0.0,
                                                       2743.68, 2776.00,
     3
                        2992.31,
     4
                       3590.86,
                                  3645.02,
                                             3693.64,
     5
                                     0.0,
                                             4367.08,
                       4223.33,
                                                       4655.205,
     6
                        4821.515,
                                     0.0,
     7
                           0.0,
                                  4939.35,
                                                       5075.344/
                                                0.0,
C
      SET ENERGY LEVELS FOR THE 638, 637, AND 828 ISOTOPES
c
      DATA (ENL2(I,5),I=1,29)/0.,643.23, 1244.93, 1286.86, 1342.37,
                          3*0.0, 2265.973, 20*0.0/
      DATA (ENL2(I,6),I=1,29)/0.,645.744, 1254.83, 1291.80, 1355.52,
      3*0.0, 2274.33, 20*0.0/
DATA (ENL2(I,7),I=1,29)/0.,657.33, 1230.33, 1315.08, 1347.097,
                         3*0.0, 2314.052, 20*0.0/
C
Č
      SET THE STATISTICAL WEIGHTS OF THE 29 CO2 LEVELS
C
      DATA (STW2(I),I=1,29)/ 1, 2, 1, 2, 1, 1, 2, 2, 2, 1, 1,
     1
     2
                               2, 1, 2, 2, 1,
                               2,
     3
     4
                               1, 2, 1,
     5
                               2, 2, 2, 1,
                               1, 2,
                               2, 1, 2, 1/
000000
                             NO VIBRATIONAL LEVEL PARAMETERS
      IDENTIFY THE NO VIBRATIONAL LEVELS
C
      DATA (NAM8(I), I=1,13)/'0','1','2','3','4','5','6','7','8','9',
                              '10','11','12'/
С
C
      SET ENERGY LEVELS FOR THE 46,56, AND 48 ISOTOPES
С
      DATA (ENL8(I,1), I=1,13)/0.0,1875.9711,3723.8526, 5543.6909,
                                     7335.5312,9099.4078,10835.3427,6*0.0/
      DATA (ENL8(1,2), I=1,13)/0.0,1842.9177,11*0.0/
      DATA (ENL8(I,3), I=1,13)/0.0,1827.2844,11*0.0/
C
C
      SET THE STATISTICAL WEIGHTS OF THE NO LEVELS
С
      DATA (STW8(I), I=1,13)/13*1/
С
C
С
C
      END
```

```
BLOCK DATA PRESS
C
      ATMOSPHERIC PRESSURE, IN ATMOSPHERES, AT ALTITUDES BETWEEN 0 AND 191
С
С
      IN 1-KM INTERVALS. DATA ARE FROM US STANDARD ATMOSPHERE, 1976.
C
      DIMENSION PR(192)
      COMMON/P/PR
С
      ALTITUDES 0-95 KM IN THE FIRST HALF OF THE ARRAY
      DATA (PR(I), I=1, 96)/
     1.10000E+01,.88700E+00,.78461E+00,.69204E+00,.60854E+00,.53341E+00,
     2.46600E+00,.40567E+00,.35185E+00,.30397E+00,.26153E+00,.22403E+00,
     3.19145E+00,.16362E+00,.13985E+00,.11953E+00,.10217E+00,.87340E-01,
     4.74663E-01,.63829E-01,.54570E-01,.46671E-01,.39945E-01,.34215E-01,
     5.29328E-01,.25158E-01,.21597E-01,.18553E-01,.15950E-01,.13727E-01,
     6.11813E-01,.10177E-01,.87743E-02,.75727E-02,.65473E-02,.56708E-02,
     7.49200E-02,.42758E-02,.37220E-02,.32452E-02,.28338E-02,.24803E-02,
     8.21709E-02,.19056E-02,.16728E-02,.14725E-02,.12962E-02,.11439E-02,
     9.10095E-02,.89153E-03,.78735E-03,.69530E-03,.61401E-03,.54121E-03,
     A.47705E-03,.41941E-03,.36873E-03,.32331E-03,.28348E-03,.24786E-03,
     B.21671E-03,.18892E-03,.16470E-03,.14314E-03,.12441E-03,.10778E-03,
     C.93372E-04,.80619E-04,.69607E-04,.59888E-04,.51526E-04,.44168E-04,
     D.37861E-04,.32350E-04,.27642E-04,.23552E-04,.20067E-04,.17762E-04,
     E.15721E-04,.12779E-04,.10387E-04,.87689E-05,.74028E-05,.62288E-05,
     F.52410E-05,.43947E-05,.36850E-05,.30852E-05,.25831E-05,.21634E-05,
     G.18119E-05,.15181E-05,.12719E-05,.10662E-05,.89375E-06,.74997E-06/
      ALTITUDES 96-190 KM IN THE SECOND HALF OF THE ARRAY
С
      DATA (PR(I), I=97, 192)/
     E.62932E-06,.52900E-06,.44468E-06,.37482E-06,.31593E-06,.26863E-06,
     I.22841E-06,.19508E-06,.16661E-06,.14310E-06,.12291E-06,.10632E-06,
     J.91970E-07,.80301E-07,.70113E-07,.61997E-07,.54821E-07,.49053E-07,
     K.43892E-07,.39661E-07,.35837E-07,.32652E-07,.29750E-07,.27299E-07,
     L.25050E-07,.23127E-07,.21352E-07,.19816E-07,.18391E-07,.17145E-07,
     M.15983E-07,.14957E-07,.13997E-07,.13143E-07,.12341E-07,.11623E-07,
     N.10947E-07,.10337E-07,.97614E-08,.92397E-08,.87459E-08,.82962E-08,
     O.78696E-08,.74795E-08,.71087E-08,.67682E-08,.64440E-08,.61453E-08,
     P.58604E-08,.55970E-08,.53454E-08,.51121E-08,.48890E-08,.46815E-08,
     R.44828E-08,.43063E-08,.41367E-08,.39738E-08,.38173E-08,.36670E-08,
     S.35<sup>2</sup>6E-08,.33839E-08,.32507E-08,.31227E-08,.29997E-08,.28937E-08,
     T.27914E-08,.26928E-08,.25976E-08,.25058E-08,.24173E-08,.23319E-08,
     U.22495E-08,.21700E-08,.20933E-08,.20257E-08,.19602E-08,.18969E-08,
     V.18356E-08,.17762E-08,.17188E-08,.16633E-08,.16095E-08,.15575E-08,
     X.15072E-08,.14620E-08,.14182E-08,.13757E-08,.13345E-08,.12945E-08,
     Y.12557E-08,.12181E-08,.11816E-08,.11451E-08,.11118E-08,.10797E-08/
С
      END
```

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